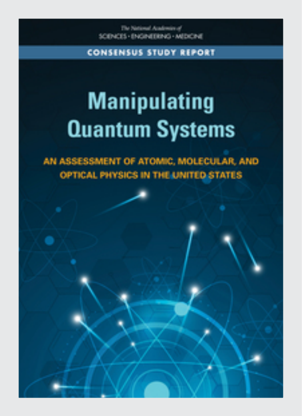

# Manipulating Quantum Systems: An Assessment of Atomic, Molecular, and Optical Physics in the United States (2020)

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# Manipulating Quantum Systems

## AN ASSESSMENT OF ATOMIC, MOLECULAR, AND OPTICAL PHYSICS IN THE UNITED STATES

Committee on Decadal Assessment and Outlook Report on Atomic, Molecular, and Optical Science

Board on Physics and Astronomy

Division on Engineering and Physical Sciences

A Consensus Study Report of

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# Preface

This report is an accounting of the "AMO 2020" decadal study undertaken by the National Academies of Sciences, Engineering, and Medicine to assess opportunities in AMO (atomic, molecular, and optical) science and technology over the coming decade. The charge for this study was devised by a Board on Physics and Astronomy standing committee, the Committee on Decadal Assessment and Outlook Report on Atomic, Molecular, and Optical Science, in consultation with the study's sponsors, the Department of Energy (DOE), the National Science Foundation (NSF), and the Air Force Office of Scientific Research (AFOSR). The main task for the committee is to provide insights for both scientists and agencies in finding opportunities to advance established and emerging areas of AMO, through funding, education, and industrial partnerships.

The Committee on AMO 2020, which carried out the study, was asked to assess the state of the field of AMO science, emphasizing recent accomplishments and identifying new and compelling scientific questions and opportunities. The committee that carried out this study and wrote this report comprised leaders from many different subfields within the AMO physics community, as well as prominent scientists from outside the field. By highlighting a summary review of the field of AMO science as a whole, the committee describes opportunities for scientific discoveries and new technological development. The report is structured around scientific grand challenges, with science goals, tool development, and research impact interleaved throughout the main science chapters. These summaries are intended as a guideline to identify the impacts of AMO science, now and in the coming decade, on emerging technologies and in meeting national needs.

The committee held five in-person meetings and numerous teleconferences among members to provide input, receive feedback, deliberate findings, and collaborate on writing. In addition, the committee received valuable input in the form of presentations from the following colleagues during some of the in-person meetings: Phil Bucksbaum, Paul Corkum, Dave DeMille, Emily Domenech, Markus Greiner, Anna Krylov, Steve Leone, Chris Monroe, Oskar Painter, Adam Rosenberg, Daniel Savin, and Jelena Vuckovic. The following individuals also provided perspective from the federal agencies: John Gillaspy (NSF/Mathematical and Physical Sciences [MPS]), Grace Metcalf (AFOSR), and Tom Settersten (DOE/Chemical Sciences, Geosciences, and Biosciences [CSGB]).

Significant effort was made to solicit community input for this study. This was done via town hall meetings held at the Annual Meeting of the Division of AMO Physics of the American Physical Society (APS) in Ft. Lauderdale, Florida, in May 2018 and the Frontiers in Optics Conference hosted by the Optical Society of America and co-sponsored by APS, Division of Laser Science in September 2018 in Washington, D.C. The committee also solicited input from the community through a public website and received many white papers. The comments supplied by the AMO community through this site and at the town hall meetings were extremely valuable primary input to the committee. The committee also consulted a number of reports concerning the connection of AMO science to photonics, quantum information, and space-related activities. The committee acknowledges valuable input from the following colleagues: Alain Aspect, Paul Baker, Louis Barbier, Lisa Barsotti, Klaus Bartschat, Scott Bergeson, Klaus Blaum, Brad Blakestad, Immanuel Bloch, Doerte Blume, Stephen Boppart, Steven Boxer, Igor Bray, Paul Brumer, Dmitry Budker, Jaime Cardenas, Jenna Chan, Ignacio Cirac, Eric Cornell, Steve Cundiff, Tatjana Curcic, Brian DeMarco, John Doyle, Francesca Ferlaino, Debra Fischer, Graham Fleming, Nathan Goldman, Barbara Goldstein, Rudolf Grimm, Christian Gross, Richard Hammond, Ulrich Höfer, Matt Hourihan, Liang Jiang, Sabre Kais, Henry Kapteyn, Wolfgang Ketterle, Thomas Killian, Derek Jackson Kimball, H. Jeff Kimble, Tobias Kippenberg, David Kleinfeld, Svetlana Kotochigova, Ferenc Krausz, Anne L'Huillier, Todd Martinez, C. William McCurdy, William Moerner, Sarah Monk, Margaret Murnane, Frank Narducci, David Newell, Kang-Kuen Ni, Tilman Pfau, Nathalie Picque, Johannes Reimann, David Reis, Ana Maria Rey, Tara Ruttley, Dan Stamper-Kurn, Marc Ulrich, Pieter van Dokkum, Vladan Vuletic, Ronald Walsworth, Andrew Weiner, Jonathan Wheeler, Tommy Willis, Norm Yao, and Linda Young.

The national organizations and federal agencies that support AMO research in the United States were also solicited for input, through their direct testimony at open meetings and their written responses to requests for information on funding patterns, demographic information, and other statistical data. These data are summarized in Chapter 8 and in the appendixes to the report. The committee is also grateful to the staff from the committees in Congress concerned with funding legislation, who provided important background on connections between AMO science and national science policy.

The AMO field continues to progress at an exciting pace for both scientific discoveries and technological innovations. The increasingly stronger and pervasive connections to many disciplines of physical and biological sciences have made AMO a cornerstone for modern science and emerging technologies, and we note particularly the fundamental role AMO plays in shaping the ongoing revolution in the field of quantum information science and technology. AMO has become a vital engine for current and future economic development. It is the collective enthusiasm and optimism of the AMO scientific community that helped make writing this report a pleasant and rewarding task. The committee gratefully acknowledges the infinite talent, expertise, and tireless efforts of our committee members, who contributed enormously to the success of this report, as well as valuable contributions from many colleagues from our community. The committee is grateful to Tom O'Brian and the National Institute of Standards and Technology for strong support for the committee activities. Last, the committee expresses its sincere gratitude to Chris Jones for his dedication, expertise, and organizational skills, to Jim Lancaster for his insights and guidance, and to the National Academy of Sciences staff for their many important contributions to data analysis during the writing of this report. The committee is also deeply grateful for the partnership between the co-chairs that made this study a fulfilling and enjoyable process.

# Acknowledgment of Reviewers

This Consensus Study Report was reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise. The purpose of this independent review is to provide candid and critical comments that will assist the National Academies of Sciences, Engineering, and Medicine in making each published report as sound as possible and to ensure that it meets the institutional standards for quality, objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process.

We thank the following individuals for their review of this report:

Philip H. Bucksbaum, NAS,[1] Stanford University,
Lincoln Carr, Colorado School of Mines,
Charles W. Clark, National Institute of Standards and Technology,
David P. DeMille, Yale University
Thomas C. Killian, Rice University,
Prem Kumar, Northwestern University,
Robert A. Lieberman, NAE,[2] Lumoptix, LLC,
Cindy Regal, University of Colorado, Boulder,
Daniel Savin, Columbia University,
Peter T. So, Massachusetts Institute of Technology, and
Linda Young, Argonne National Laboratory.

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[1] Member, National Academy of Sciences.

[2] Member, National Academy of Engineering.

Although the reviewers listed above provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations of this report nor did they see the final draft before its release. The review of this report was overseen by Julia M. Phillips, NAE, Sandia National Laboratories, and David J. Wineland, NAS, University of Oregon. They were responsible for making certain that an independent examination of this report was carried out in accordance with the standards of the National Academies and that all review comments were carefully considered. Responsibility for the final content rests entirely with the authoring committee and the National Academies.

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APPENDIXES

# Summary

From navigation and time-keeping to health and medical care, the field of atomic, molecular, and optical (AMO) physics has provided numerous important scientific and technological advances that have transformed human society in the past several decades. Harnessing the exquisite quantum properties of atoms and their interaction with light underpins many everyday technologies—from the lasers in consumer electronics, medical technologies such as laser therapies, and magnetic resonance imaging (MRI), to the most precise atomic clocks, which maintain the accuracy of the global positioning system. Within the past decade alone, the techniques of AMO physics played a pivotal role in the discovery of gravitational waves and the new era of multimessenger astrophysics that is ensuing, and in the explosive development of quantum information and sensing technologies.

AMO physics studies the fundamental building blocks of matter to help advance the understanding of the universe. It is a foundational discipline within the physical sciences, relating to atoms and their constituents, to molecules, and to light at the quantum level. AMO physics combines fundamental research with practical application, coupling fundamental scientific discovery to rapidly evolving technological advances, innovation, and commercialization.

Because of the wide-reaching intellectual, societal, and economical impact of AMO, agencies within the federal government have deemed it worthwhile to conduct a survey of the recent advances in AMO physics, and to review what may be on the horizon for the field. This report reflects on the successes of AMO science and identifies the most pressing current challenges, as well as the most promising future opportunities presented by AMO science. The U.S. research community has long enjoyed global leadership in AMO physics, thanks to sustained, strong support from the federal government and the unique AMO culture that fosters collaboration and open research. At the same time, the broader international scientific community has recognized the importance of AMO research, and over the past decade the U.S. global leadership position has begun to erode, as funding has not kept up with growth in the field, and other countries have increased investments in this field. As such, this report also considers federal funding trends and practices, trends in education and workforce participation, and ways to ensure the continued health of AMO science in the United States and globally.

The committee's advice is summarized into 10 broad and high-level recommendations, which are directed at the entire AMO research enterprise and are highlighted at the end of this summary and in the Overview of Chapter 1. The committee provides another 16 more focused, subfield-specific recommendations, embedded within the relevant chapters, which are also summarized in Chapter 1.

## FUNDING

Considering the breadth and depth of AMO physics described above, the committee strongly urges continued national investment in AMO science; as a curiosity-driven research enterprise it has been the driving force behind many scientific discoveries and innovative technologies. Given the central role of AMO science to other disciplines in physical sciences, and considering the increasingly large investments in AMO-related quantum information science and technology in European countries and China, coordinated interagency support is needed for continued development and leadership of AMO science in the United States. Within the United States, data collected from three agencies that fund AMO science—the National Science Foundation (NSF), the Department of Defense (DoD), and the Department of Energy (DOE)—shows that aggregate funding over the past decade for AMO science has not kept up with the growth of the field, showing large annual variations for certain programs, and essentially flat budgets for others.

> **Key Recommendation: The U.S. government should vigorously continue investment in curiosity-driven atomic, molecular, and optical (AMO) science to enable exploration of a diverse set of scientific ideas and approaches. AMO is a critical investment in our economic and national security interests.**

Noting important discovery potentials, current funding situations, and international competitiveness, the committee finds specific opportunities in certain research areas and for certain funding agencies, many of which are discussed in the findings presented in Chapter 1. AMO and quantum science continues to improve necessary precision measurement concerning fundamental physics, and has produced significant discoveries in the area traditionally the realm of particle physics. Thus, AMO-based projects on quantum sensing and addressing beyond-the-standard-model fundamental physics questions will be key in meeting emerging opportunities in quantum science.

The development of quantum technologies brings important new opportunities in sensing and precision measurement that can have applications ranging from quantum computation and simulation, enhanced communication and navigation, to fundamental probes of the universe. With quantum information technology still at a very early stage, there is an increasing number of potential new systems and platforms one can exploit for the construction of quantum machines. Therefore, it is urgent that the research community develop platform-independent metrics to measure and characterize the performance of quantum technologies. Nurturing research into quantum information systems, work that will provide critical tools and insights for other areas of science, will require long-term investments that cross traditional disciplinary boundaries.

**Key Recommendation: Basic research in science, engineering, and applications underlying both existing and emerging new platforms needs to be broadly supported, including research on techniques for cross-verification of quantum machines across different platforms for various applications. Specifically, the committee recommends that the National Science Foundation, Department of Energy, National Institute of Standards and Technology, and Department of Defense should provide coordinated support for scientific development, engineering, and early applications of AMO-based quantum information systems.**

Rapid advances in the precision and capabilities of AMO technologies have dramatically increased the potential of AMO-based techniques to discover new physics beyond the standard model. The present lack of a federal funding program dedicated specifically to supporting such research at the intersection of high-energy physics and AMO is a limiting factor in fully utilizing the plethora of opportunities for new discoveries.

**Key Recommendation: The Department of Energy's High-Energy Physics, Nuclear Physics, and Basic Energy Sciences programs should fund research on quantum sensing and pursue beyond-the-Standard-Model fundamental physics questions through AMO-based projects.**

Armed with emerging AMO technologies, both space- and laboratory-based fundamental AMO science is needed to address key questions in astronomy, astrophysics, and cosmology. Likewise, the committee finds that the time is ripe for recently developed AMO tools and technologies to be deployed in space missions.

> **Key Recommendation: The National Aeronautics and Space Administration, in coordination with other federal agencies, should increase investments in theory and experiment for both space- and laboratory-based fundamental atomic, molecular, and optical science that are needed to address key questions in astronomy, astrophysics, and cosmology.**

Creative science carried out by single principal investigator (PI) groups is the heart of AMO science. The field has done well building on the innovative, imaginative efforts of these individual investigators, but it is entering a new phase for which collaborations with flexible-sized teams would enable exciting new discoveries that may call for focused efforts. Advances in ultrafast light sources will be key to microscopic understanding of dynamics in complex systems, such as the motion of electrons in a material. Therefore, it is important to continue investment in a broad range of science, including at ultrafast X-ray light source facilities, while maintaining a strong single PI funding model. The 2018 National Academies report *Opportunities in Intense Ultrafast Lasers: Reaching for the Brightest Light* recommended that the DOE lead the development of a comprehensive interagency strategy for high-intensity lasers that includes the development and operation of both large-scale national laboratory projects and mid-scale university-hosted projects. A good balance between facilities and single-investigator programs in the context of emerging quantum centers is particularly important.

> **Key Recommendation: U.S. federal agencies should invest in a broad range of science that takes advantage of ultrafast X-ray light source facilities, while maintaining a strong single principal investigator funding model. This includes the establishment of open user facilities in mid-scale university-hosted settings.**

## EDUCATION AND WORKFORCE DEVELOPMENT

Academia needs to evolve to encourage cross-disciplinary hiring of both theorists and experimentalists at the rapidly growing interfaces between AMO and quantum information science, computer science, mathematics, chemistry, biology, astrophysics, engineering, and industry. Overall, education in preparation for a research career, measured by the number of Ph.D.s granted, remains robust. In order for other fields to be able to take advantage of critical AMO advances, it is important to improve educational programs and funding mechanisms that encourage interdisciplinary work/collaboration to translate AMO work across fields.

Strong collaboration between theorists and experimentalists has been important for maintaining the health of AMO science. However, the number of faculty positions in AMO theory has been limited. Additionally, experimental AMO science has become very expensive, and the starting cost of a new experimental program has become a deterrent for young AMO scientists being appointed as faculty in academia. The translation from AMO science to technology and engineering and a strong partnership between AMO academia and industry are particularly important now with the national emphasis on the development of quantum technologies and a corresponding new generation of workforce.

AMO technologies are not being transferred into other fields for use as rapidly as AMO science itself develops. The committee finds that it is increasingly important to improve the visibility of AMO. The breakneck pace of AMO breakthroughs leads the committee to believe that other communities would benefit from knowing more about AMO. Furthermore, departmental boundaries create barriers for young AMO-trained post-docs to move into related disciplines and departments, such as quantum information science and computer science, where their AMO training would play key roles in advancing those fields. In particular, quantum technology cuts across scientific fields and technologies beyond AMO, and so encounters barriers with traditional funding mechanisms. Recent Quantum Leap Initiatives at NSF are based on a stewardship model that starts to break the traditional barriers between disciplines.

Traditional AMO training focuses on physics; however, the development of quantum technology requires reaching across both academic disciplines and to industry to leverage the impact of AMO. There are existing successful portable funding models in the United States and Europe, such as the National Institutes of Health (NIH)-K99 and European Research Council (ERC) grants, that could be used as models to assist faculty appointment and early career development. In designing such portable funding models, it will be important to ensure that the level of research effort is compatible with teaching expectations that are standard in the physical sciences academic community. Other AMO funding agencies should develop similar models that support the transition of AMO theorists and experimentalists into faculty positions.

**Key Recommendation: AMO funding agencies should develop portable fellowship grant models that support the transition of AMO science theorists and experimentalists into faculty positions.**

**Key Recommendation: To maximize the effectiveness of federal investment, academia should enable and encourage cross-disciplinary hiring of theorists and experimentalists at the rapidly growing interface between AMO science fields and computer science, mathematics, chemistry, biology, engineering, as well as industry.**

> **Key Recommendation: The National Science Foundation, Department of Energy, National Institute of Standards and Technology, and Department of Defense should increase opportunities for translating atomic, molecular, and optical science advances to other fields by fostering collaboration with scientists and engineers from other disciplines through, for example, support of workshops and similar mechanisms for cross-disciplinary interactions.**

AMO science, like other physics disciplines, continues to have difficulty in attracting women and underrepresented minorities at all levels. It is clear that education and workforce development in AMO is not keeping up with the demographics in the nation, and that this is a lost opportunity. There is a growing untapped national talent pool of women and underrepresented minorities.

> **Key Recommendation: The entire AMO science enterprise should find ways to tap into the growing national talent pool of women and underrepresented minorities. The committee therefore endorses the relevant recommendations in the National Academies reports *Graduate STEM Education for the 21st Century* and *Expanding Underrepresented Minority Participation*, for example.**

## INTERNATIONAL CONNECTIONS OF ATOMIC, MOLECULAR, AND OPTICAL SCIENCE

The health of AMO science relies heavily on strong international collaborations, and this report identifies regulatory impediments to fostering international collaborations and maintaining U.S. leadership in research, education, and innovation globally (see Chapter 8). Yearly trends of research publications provide a good indicator that the United States maintains a strong position in AMO science globally, although many European nations, China, South Korea, Japan, and Australia are rapidly catching up or already leading in certain subfields of AMO. Mechanisms for co-funding research that is carried out with international collaboration fuels collective progress in AMO science. However, the committee finds that the U.S. position in terms of investment and commercialization in this area has weakened compared to Europe and Asia. There are a number of technical and regulatory impediments including major differences in effort certification, intellectual property ownership policies, and conflict-of-interest rules, as well as unfunded external audit requirements and unreasonable currency exchange requirements, all of which make it difficult for U.S. universities to accept and administer grants from, for example, the European Union (EU).

The committee recognizes the real security concerns in open, international collaboration, but there is great national benefit in having intellectual leaders visiting the United States. This benefit is at risk due to continuing significant issues with access to national research facilities, and visa denials and excessive delays for international students, collaborators, and speakers at conferences. Open collaborations have been vital for the health of AMO physics, and the nation's reputation as a welcoming place for the best international students and researchers has been key to attract future leaders to the United States. The Office of Science and Technology Policy and federal funding agencies need to work collaboratively with the Department of State and an academic consortium such as the Council on Governmental Relations to remove impediments to international cooperation.

> **Key Recommendation: The committee recognizes the real security concerns in open, international collaboration. However, because open collaborations have been so vital for the health of atomic, molecular, and optical physics, the Office of Science and Technology Policy and federal funding agencies should work collaboratively with the Department of State and an academic consortium such as the Council on Governmental Relations to remove impediments to international cooperation. There is a critical need for**
>
> 1. **Blanket agreements for funding agencies in different countries to accept each other's grant administration regulations;**
> 2. **Standardized mechanisms for joint funding of cooperative projects; and**
> 3. **Mechanisms to remove excessive visa application delays for international students, collaborators, and speakers at U.S. conferences and workshops.**

## IMPORTANT TOPICS IN AMO PHYSICS

This report highlights major scientific themes that are of strong current interest and have substantial growth potentials for AMO science, presenting them in Chapters 2 to 7. These grand challenge themes are closely related, and their interconnections highlight the richness and expansiveness of AMO science.

- *Chapter 2: Tools Made of Light.* The strong tradition in advancing the frontiers of light properties and creating new platforms with light will be a key part of AMO to enable future progress in fundamental discoveries and novel technologies. Generating light with precisely controlled properties has enabled novel tools for probing and controlling matter, providing greater reach into the unique phenomena underlying fundamental physics.
- *Chapter 3: Emerging Phenomena from Few- to Many-Body Systems.* Microscopic control of a diverse set of atoms and molecules at the quantum level is a critical foundation of AMO from which new scientific understandings emerge and new toolboxes are created. The committee explores atomic and

molecular systems where scaling from a few particles to many reveals new phenomena that emerge due to the quantum interactions between atoms.

- *Chapter 4: Foundations of Quantum Information Science and Technology*. As AMO provides one of the most precisely controlled quantum systems that form the basis for quantum information processing, AMO will play a central role in delivering the most promising approaches in this increasingly active field. The production, transmission, storage, and use of quantum bits (qubits) are the building blocks of quantum information systems that promise computational and encryption advantages exceeding the capabilities of current classical computing.
- *Chapter 5: Harnessing Quantum Dynamics in the Time and Frequency Domains.* Novel tools of light and matter are providing unprecedented clarity in the observation and understanding of how systems evolve at vastly different time scales and across a large range of energies, creating new opportunities for controlling matter. Studying the dynamics and transformations of quantum systems on varying time scales provides extraordinary opportunities to create, manipulate, and understand quantum matter.
- *Chapter 6: Precision Frontier and Fundamental Nature of the Universe.* AMO-based technologies are being deployed to solve some of the outstanding scientific puzzles of our time, including the study of fundamental symmetries, testing physics postulates, searches for dark matter, and the detection of gravitational waves. Through the precise control of light, atoms, and molecules, the tools of AMO science have become integral to the exploration of fundamental phenomena in nature. The precision achievable by AMO techniques, coupled to and cross-fertilized by different disciplines of physics, will play a leading role in understanding nature at the deepest and most fundamental level.
- *Chapter 7: Broader Impact of AMO Science.* Because of its deep connections to other scientific disciplines and to advanced engineering and industrial innovations, the impact of AMO on scientific discovery and technological progress extends over a wide swath of human society—from life and health sciences to material engineering. A natural consequence of the sheer breadth and diversity of AMO tools and techniques is their applicability to many scientific endeavors outside the traditional boundaries of AMO science. These connections in turn fuel creative ideas and new developments within AMO.

# 1

# Manipulating Quantum Systems: AMO Science in the Coming Decade

## INTRODUCTION AND OVERVIEW

Atomic, molecular, and optical (AMO) physics is a foundational discipline within the physical sciences. It is the study of light and matter and their interactions, and deals with electrons, atoms, molecules, and light at the quantum level. These are the fundamental building blocks of matter and their quantum-level behavior provides us fundamental understanding of the universe. At the same time, AMO is also of paramount importance for providing critical technological infrastructure for economic development, national security, and future human endeavors. These complementary features—spanning from very fundamental to very practical—provide a unique character to AMO physics, namely the rapidly evolving, strongly coupled cycles between scientific discovery and technological advances. Another powerful feature of AMO science is that it often provides the best—and sometimes, the only—viable platform to achieve certain scientific or technological goals, such as in the areas of sensing and metrology. As a consequence, the prominence of AMO physics in the scientific arena has continued to grow significantly in recent times. Atoms, molecules, and photons—all under precise control while interacting and interconnecting in the quantum regime—play decisive roles in shaping our understanding of the basic laws of nature. This control now enables researchers to manipulate quantum systems in order to tackle outstanding problems in the complexity of matter, to probe the elusive secrets of nature, and at the same time to give birth to new technologies that transform human society. In this way, AMO science offers deep and ubiquitous connections between fundamental science and applied technologies.

The historical perspective of AMO is telling. Efforts in AMO (or more traditionally, spectroscopy) led to the birth of quantum mechanics more than 100 years ago. Since that time, AMO has remained at the forefront of testing some of the most fundamental laws of nature, has stimulated the emergence of new scientific disciplines, and has provided increasingly sophisticated technical infrastructure for modern society. Today, AMO is leading the way for a renaissance of quantum physics, promising a new revolution in information processing and metrology.

A historical strength of the AMO culture is the invention, development, and construction of cutting-edge research tools, including, for example, the invention of lasers and the development of quantum information processing platforms. Another unique aspect is unusually strong close collaborations between experiment and theory. These aspects of the culture allow AMO science to open many new windows to explore deeper scientific questions, and at the same time provides a key technological underpinning for economic development. For two major U.S. National Initiatives that have emerged recently—the National Photonics Initiative and the National Quantum Initiative (NQI)—AMO science serves as the cornerstone for the foundational technologies, and the key drive to economic impact, which includes workforce training, education, industry connections, and product development.

When it comes to the ability to control physical systems—down to the level of individual quanta—AMO technology is the unchallenged leader. This ability is conducive to extracting both a rigorous understanding and the universal features from particular physical systems, and it also provides the basis for tackling increasingly more complex problems. Control, as an enabling capability, provides a natural approach for building physical understanding, and from which to design systems from the ground up. Not surprisingly, precision control also provides illuminating guidance for top-down analysis and system construction. The now pervasive control of simple quantum systems starts from single photons and single atoms and molecules. Building from there, this control has provided a rich arena for AMO scientists to tackle both systems that are more complex and more strongly interacting. This capability has, for example, been crucial to the development of the basic infrastructure for the emergence of quantum information science (QIS). Control allows bridging the gap from few- to many-body physics, and understanding and manipulating quantum coherence, complexity, and dynamics. Together these features position AMO to drive the next revolution in measurement that could provide answers to some of the most fundamental questions concerning physics, and could offer new opportunities to explore grand challenges in both science and technology.

As previously suggested, AMO is strongly positioned among all disciplines of the physical sciences in that it plays a central role in connecting intellectual frontiers and technological foundations. It does so not just within AMO physics, but broadly. It does this for astrophysics; condensed-matter, plasma, high-energy, particle, and nuclear physics; gravitation and cosmology; chemistry; biology; and health. It is a key driver behind the quantum information revolution. Numerous AMO researchers have garnered international recognition for their accomplishments, the annual Nobel Prize being perhaps the most universally revered. Since 2004, the time of publication of the previous decadal study, 20 scientists have been awarded Nobel Prizes in Physics for research that related to AMO science. These include Ashkin for optical tweezers and applications to biological systems (2018); Mourou and Strickland for generation of high-intensity, ultrashort optical pulses (2018); Weiss, Thorne, and Barish for the observation of gravitational waves (2017); Akasaki, Amano, and Nakamura for the invention of blue light emitting diodes, which has enabled bright and energy-saving white light sources (2014); Haroche and Wineland for methods that enable measuring and manipulation of single quantum systems (2012); Kao for transmission of light in fibers for telecommunications (2009); Boyle and Smith for the invention of an imaging semiconductor circuit—the charge-coupled device sensor (2009); Glauber for the quantum theory of optical coherence (2005); and Hall and Hänsch for precision spectroscopy and optical frequency combs (2005). The reach of AMO science is felt beyond physics, and indeed the 2014 Nobel Prize in Chemistry was awarded to Betzig, Hell, and Moerner for the development of super-resolved fluorescence microscopy.

In addition to the Nobel Prize, the Kavli Prize, the Breakthrough Prize, and the Wolf Prize are symbols of recognition of scientific eminence. Here too, AMO science has fared very well, with nearly a dozen prize recipients recognized for AMO-related science in the past decade.

Perhaps the biggest international recognition for AMO research is the widespread support for AMO among all leading industrialized countries, including rising national funding and improved educational efforts. The purpose of this report is to reflect on these successes, and to identify the most pressing current challenges as well as the most promising future opportunities in AMO science.

In this spirit, the committee structures this decadal report to highlight the scientific achievements from the past decade, and to identify the great opportunities that lie ahead in the field of AMO sciences. These include scientific discoveries within AMO and a wide range of applications that will be based on them. The committee outlines six major scientific themes that form the core of AMO science, presented in the following six chapters: “Tools Made of Light,” “Emerging Phenomena from Few- to Many-Body Systems,” “Foundations of Quantum Information Science and Technology,” “Harnessing Quantum Dynamics in the Time and Frequency Domains,” “Precision Frontier and Fundamental Nature of the Universe,” and “Broader Impact of AMO Science.”

These six closely connected grand challenge themes represent numerous recent scientific accomplishments and key scientific opportunities. Each theme discussion contains three components—fundamental science, technological development and tools, and broad impact. A tool developed under one theme may enable the exploration of science in another, which in turn may open powerful applications in a third theme. As a result, there is strong overlap across chapters in terms of both science and technological tools. This theme-oriented structure for this report differs from a more traditional categorization of individual areas of the AMO field, such as ultracold, ultrafast, or ultraprecision physics. Instead, the committee integrates these traditionally identified areas, which then permeate the entire report through the multiple scientific themes. For example, a reader who is an expert in the control of light will find relevant discussions of his or her work in chapters where it is the main subject of research, and also in chapters where it provides essentials tools for quantum state control and precision measurement, and yet in other chapters where new physical systems provide novel opportunities with their light sources. The discussion on ultracold matter centers on emerging phenomena in many-body systems, and provides an intimate connection to QIS. Below, the committee briefly outlines each of the six scientific themes that are presented in this report. Interconnected together, the goal is for these six themes to form a coherent overview of AMO science, and for the reader to appreciate the universal connections between scientific vision and technology development within AMO.

## CHAPTER 2: TOOLS MADE OF LIGHT

The invention of new light sources has always been a path toward obtaining deeper understanding of the physical world, from seeking its finer structure to following more rapidly changing behaviors. Further, the development of light sources is, in itself, a scientific venture that requires utmost control of atoms and molecules, accelerated electrons, collective states of atoms, and solid-state environments. The field of AMO seeks to create and harness a variety of new light sources that advance multiple metrics for the control of electromagnetic radiation: ultrashort light pulses from the extreme ultraviolet (XUV) to the X-ray domain, extreme high-intensity laser fields, highly nonclassical light, and extremely coherent light, as examples. These light sources, each specifically tailored for corresponding scientific explorations, allow researchers to advance the frontiers of spectroscopy, to establish new networks including quantum communications and computing, and to explore phenomena that occur under the extreme conditions of ultrahigh fields or at ultrashort time scales. At the same time, the integration of light and matter, in the form of novel nanophotonic structures or large-scale interferometers as just two examples, provides the next technological frontiers for manufacturing mass-scaled and transportable devices.

## CHAPTER 3: EMERGING PHENOMENA FROM FEW- TO MANY-BODY SYSTEMS

By precisely probing the microscopic underpinnings of emergent phenomena in quantum matter, interacting, many-body quantum systems can be studied and understood. In this process, new insights are gained into the emergence of universal rules that govern complex materials and inspire novel quantum measurement approaches for exploring unknown corners of our physical world. On the one hand, an interacting many-body quantum system presents fundamental challenges to the understanding of its properties. On the other hand, once understood and controlled, such a system turns into a tool for fundamental gains in measurement and information processing, at the same time expanding the range of science and creating new technology.

To provide the enabling technical capabilities and key insights to the emergence of complexity, researchers need to build quantum matter from well-controlled quantum particles and excitations, from constituents ranging from photons, atoms, molecules, and nano-quantum components. A common theme is the ability to gather many constituents while still accessing measurement at the single-particle level. Second, we need to understand and manipulate interactions between individual quantum particles, through the use of key ingredients such as time-dependent drives, engineered reservoirs, controlled geometry and topology, disorder and frustration, and quantum entanglement. The realization of new forms of quantum matter advances our understanding of complex quantum behavior and provides guiding principles for discovery of advanced materials and novel technologies. Furthermore, precisely controlled quantum systems that are necessary for this line of research provide natural platforms for quantum information processing, a subject for the following chapter discussion.

## CHAPTER 4: FOUNDATIONS OF QUANTUM INFORMATION SCIENCE AND TECHNOLOGY

The production, transmission, and use of quantum bits (qubits) offer tremendous promise for computation, simulation, communication, sensing, and network performance beyond current technological limits. Very likely, quantum information processing (QIP) will rely on multiple platforms, each with different strengths and shortcomings, for storing, manipulating, and transporting quantum information. Great opportunities and challenges exist in parallel. On the one hand, open questions related to the fundamentals of QIS still need to be explored and addressed; on the other hand, a range of novel QIP tools and techniques based on precisely controllable and measurable quantum systems need to be developed now to foster the growth of quantum technology.

AMO systems, including ultracold neutral atoms and molecules, trapped ions, and quantum states of light, have been essential for the development of all areas of quantum information science and technology (QIST). Optical lattices or tweezers filled to unity with ultracold atoms, and soon also molecules, constitute large arrays of perfectly identical qubits, in which quantum information can be stored in hyperfine or other internal states with essentially unlimited energy relaxation times, each of which can be addressed and measured with optical microscopy. Tightly focused optical traps provide a new and rapid means to assemble such quantum-bit arrays. Linear chains of identical trapped ions were among the first systems with which to realize digital quantum computing, and feature very high controllability and gate fidelity. Quantum optical systems provide resources for the transmission of quantum information and for quantum-secure communication. Neutral atom and trapped ion platforms allow for large-scale quantum simulation, with particular application to studying quantum effects in materials, and giving unprecedented experimental access to the non-equilibrium dynamics of quantum systems. The high level of control over quantum coherent states in AMO systems finds immediate application in sensing and precision measurement. It is through such applications that the present-day, less than 100 percent fidelity, and intermediate-scale quantum technologies may have their greatest impact, both in fundamental science and in a wide range of technologies.

AMO science will continue to play a leading role in this exciting research direction. To broadly advance the goals of QIP, a number of important technological developments must take place simultaneously. Although "technological" in thrust, all still require significant scientific development as well. These scientific explorations and technological developments will prepare the scientific community to further our understandings of foundational quantum physics and build an advanced QIS infrastructure consisting of the following:

- Communication, to guarantee secure data transmission and long-term security for information using entanglement-based, resilient, distributed quantum networks;
- Computation, to solve problems beyond the reach of current or conceivable classical processors by using programmable, high-fidelity quantum machines;
- Simulation, to understand and solve important problems—for example, chemical processes, new materials, as well as fundamental physical theories, by mapping them onto controlled quantum systems in an analog or digital way;
- Sensing and metrology, to achieve unprecedented sensitivity, accuracy, and resolution in measurement and diagnostics by coherently manipulating quantum objects.

## CHAPTER 5: HARNESSING QUANTUM DYNAMICS IN THE TIME AND FREQUENCY DOMAINS

A key scientific goal is to observe the dynamics and transformations of different forms of quantum matter on their natural time scales, spanning more than 10 orders of magnitude. These out-of-equilibrium dynamics often involve or create strong correlations and entanglement, and can be exceedingly difficult to observe and understand, owing to the daunting need to develop new investigative tools in both experiment and theory. This represents a grand challenge for both scientific and technological applications.

At the ultrafast time scale, molecular movies that can resolve chemical and biological transformations from the fastest electron dynamics through the relatively slower structural changes and chemical transformations offer the promise of gaining fundamental insights as well as developing biochemical applications. Furthermore, the control of coherent, subfemtosecond electron dynamics in molecules and solids can reveal and change important material characteristics, and at the same time have implications for information processing technology. The exploration of these dynamics is enabled by frontier light sources that yield femtosecond and subfemtosecond pulses spanning the infrared to the hard X-ray spectral range. With full control of the light field's amplitude, phase, and temporal structure, high-energy light sources provide an ideal tool for many powerful applications, including capturing the fastest electron dynamics in matter and helping reveal how electron scattering and screening occur on subfemtosecond time scales.

Transformational dynamics can occur at very different time scales, even though they could be governed by the same underlying physics, from the ultraslow (like the cold atoms discussed in Chapter 3) to the ultrafast (Chapter 5), and its probing via time-resolved spectroscopy thus provides a point of connection between different themes in this report. For example, the combination of molecular quantum-state control (Chapter 3) and frequency comb spectroscopy (Chapters 2 and 5), with its simultaneous high resolution in both time and frequency, permit direct and real-time detection of chemical species that provide an invaluable link to the fundamental understanding of reaction kinetics.

## CHAPTER 6: PRECISION FRONTIER AND FUNDAMENTAL NATURE OF THE UNIVERSE

AMO-based measurement science has advanced our fundamental understanding of the physical world, but, perhaps surprisingly, the deepest secrets of our universe are still waiting to be discovered. A major scientific theme within AMO is the ability to engineer new quantum systems to provide the next generation of measurement techniques to search for new physics. Additionally, foundations of quantum mechanics can be explored in simple AMO-based table-top experiments and basic models. By taking advantage of AMO techniques and fundamental understandings gained from quantum-controlled states and correlations, we turn them into quantum resources for advancing measurement sciences broadly. New table-top AMO experiments will be devised, and existing ones advanced to the next performance frontiers. These advances will probe fundamental science that complements existing approaches in high-energy, particle, and astrophysics.

The scale and discovery potential of the AMO effort to search for new physics have increased dramatically over the past decade. AMO fundamental physics now encompass a wide array of diverse experiments, including searches for permanent electric dipole moments, tests of the fundamental symmetries such as charge, parity, and time (CPT) and Lorentz symmetry; searches for variations of fundamental constants; studies of parity violation; tests of quantum electrodynamics; tests of general relativity and the equivalence principle; searches for dark matter, dark energy, and extra forces; and tests of the spin-statistics theorem. This progress is expected to accelerate in the coming decade, armed with development of new technologies, advances in AMO theory, and plentiful ideas for new searches.

AMO science also plays an important role in astrophysical probes of the universe, such as the recent discoveries of gravitational wave sources with the precision interferometers of the Laser Interferometer Gravitational-Wave Observatory (LIGO) and Virgo. With important discovery potential for the detection of new forces and in establishing new observatories for the universe based on AMO technologies, it is time for the scientific community to consider more seriously the potential of AMO in space. Access to space and microgravity is a unique tool for AMO science that enables both higher precision measurements and the possibility to carry out experiments that are impossible on Earth. The United States played an early leadership role for experiments in space with the 1992 Lambda Point Experiment that used superfluid helium onboard STS-52 to probe the renormalization group theory of phase transitions. Recently the National Aeronautics and Space Administration (NASA) has invested a large effort in establishing a Cold Atom Laboratory on board the International Space Station. Other nations have now caught up to the United States in this arena and have exceeded our capabilities in some regards. Conducting AMO research in space should also lead to key technological advances such as placing quantum sensors in orbit for navigation and establishing a quantum communication network.

## CHAPTER 7: BROADER IMPACT OF AMO SCIENCE

AMO has played and will continue to play a central role in providing inspirational scientific insights and enabling capabilities for other areas of scientific and technological development. These areas range from fundamental physics to other subdisciplines within physics, as well as to chemistry, biology, and material science, to advanced manufacturing and engineering, and to workforce training and industrial partnership. The connections between AMO and other fields foster forward-looking and synergistic research directions. While sometimes it is useful to distinguish projects that are within the AMO field's central scope from those that are not, such boundaries must be permeable, to enhance the bidirectional flow of ideas, to enable AMO to evolve in response to new developments in other areas of science, and to maximize our field's potential broader impact. As examples, AMO science has both known and unexplored applications to biological systems, to astrophysics, to plasma, nuclear, and high-energy physics, and to quantum and classical information technologies. These connections must be nurtured while not losing focus on the core missions of AMO science.

Another critically important "broader impact" concerns connections to industry, and education of the next generation of a workforce capable of advancing our increasingly technological modern society. AMO has traditionally worked hand in hand with industry to improve the performance of components used in advanced experiments while also providing innovative commercial opportunities. Manufacturers of lasers, optics, and photodetectors have contributed to the advanced AMO experimental platforms with unprecedented precision and control. These systems have in turn stimulated the development of practical sensors, industry standards, and metrological instrumentations.

## CHAPTER 8: AMO SCIENCE: PART OF THE U.S. ECONOMIC AND SOCIETAL ECOSYSTEM

Chapters 2 through 7 highlight the amazing achievements of AMO science over the past decade, and identify opportunities for scientific discoveries and new technological development in the coming decade. In doing so, the committee provides a summary review of the field of AMO science as a whole, and uses case studies in selected, nonprioritized sub-disciplines in AMO science to describe the impact that AMO science has on other scientific fields. The structure of the report is designed to help readers to readily identify scientific grand challenges, with science goals, tool development, and impact all interleaved throughout the chapters. This allows identification of opportunities and challenges associated with pursuing research in specific fields as well as in interdisciplinary areas. Additionally, these summaries provide a guideline to identify the impacts of AMO science, now and in the near future, on emerging technologies and in meeting national needs.

Following these brief summaries of the six technical chapters, the committee next turns to discuss one of the main goals of this report, which is to provide insights for scientists and federal agencies alike in exploring opportunities to advance both established and emerging areas of AMO, through funding, education, and industrial partnerships, and so on. Of course, the foremost observation is that past achievements lay the foundation for new discoveries.

AMO science does not, however, get done in isolation from the economic and societal structures in which the community operates. Chapter 8 examines the state of the field of AMO science in relation to these structures, and addresses issues of funding, workforce development, and demographic challenges. We also draw attention to the growing concerns about increasingly restrictive U.S. immigration policies and the threat to healthy international collaboration. These issues are, of course, not independent of each other, and the committee tries to make connections when possible. Through the data the committee have collected and analyzed, and by sharpening our findings and recommendations, the committee sought to address the following components of the statement of task below, and in more detail in Chapter 8:

- Evaluate recent trends in investments in AMO research in the United States relative to similar research that is taking place internationally, and provide recommendations for either securing leadership in the United States for certain subfields of AMO science, where appropriate, or for enhancing collaboration and coordination of such research support, where appropriate;
- Identify future workforce, societal, and educational needs for AMO science;
- Make recommendations on how the U.S. research enterprise might realize the full potential of AMO science.

## AMO SCIENCE AND NATIONAL POLICIES: CONCLUSIONS AND RECOMMENDATIONS

Continued advances in the grand challenges identified in this report, and in the broader frontier of AMO science generally, will rely on a number of key factors.

The first key issue is the education of the next generation of AMO scientists. We must strive to stimulate and nurture students' interest in AMO from early stages of their studies. For talented young researchers, we should provide ample opportunities to foster their emergence as the next AMO leaders. Considering the shifting societal demographics, another important question to address is how to further diversify the future AMO workforce to include the largest possible talent pool. To facilitate the development of practical applications and technology transfer, effective workforce training and industry partnership must be considered and implemented.

In order to ensure that opportunities in AMO sciences are accessible to and benefit from a diverse set of practitioners, the committee strove to examine the level of participation of women and underrepresented minorities. The committee has thus collected available data from the professional societies and from the federal funding agencies that fund or support AMO research. It was not possible to get accurate data in some cases. The lack of data on demographic trends in AMO funding and education—whether the data were not collected or were not made available for this study—was a significant impediment in addressing certain elements of the Statement of Task. Whenever available, these data have been used to infer education, professional development, and funding opportunities for women and underrepresented minorities.

Other important issues pertaining to the entire AMO field include examining the balance of support for theory and experiment. A tremendously successful ingredient in AMO has been the strong collaboration between experiment and theory. It is already part of the AMO culture that some scientists who are expert experimentalists are also excellent theorists, and theorists actively participate in experimental designs and data analysis. If the expertise and excellence in each area, and the collaboration between them, can be further strengthened, then AMO will be well poised for the challenges of the coming decade.

Another critical balance that needs careful consideration is between table-top and large-scale experiments. Nimble, small-scale experiments are the historical trademark for AMO. However, AMO did give rise to some large-scale science historically. Today we are facing unprecedented opportunities to take on some of the biggest questions in science, based on AMO approaches. Some of these require larger-scale collaborations rather than the typical table-top experiments, such as searches for new physics beyond the standard model or gravitational wave detection. The committee believes that these new opportunities should be encouraged and supported, as they have the potential to lead to groundbreaking discoveries at an accelerated pace. As pointed out in Chapter 6, the connection between AMO science and space environments should also be established with renewed enthusiasm and strong support, as there are tremendous opportunities here.

The rapid progress in AMO science is the direct result of strong investments made by the federal government's research and development agencies in the work of AMO researchers. To gauge the impact of federal funding on AMO research, and to find ways to further enhance its effectiveness, the committee also sought answers to questions on funding trends and distributions. These are presented in detail in Chapter 8. However, the committee notes here that data are collected in different ways at different agencies, and even the definition of AMO is not the same throughout. As a result, the committee was somewhat limited in the scope of the conclusions it has been able to draw.

AMO science has been pursued in academia, national laboratories, and industry, and it has been greatly enhanced by collaborations between these different research venues. The committee also found it important to explore and understand interagency activities and partnerships to strengthen such collaborations, especially in areas where grand challenge problems are to be tackled. For example, the National Science Foundation (NSF), National Institute of Standards and Technology (NIST), and Department of Energy (DOE) are discussing how to work together on quantum information–related initiatives, where it will be important to combine resources and strengths to advance a few key breakthroughs in quantum technology. International connections and collaborations have historically played a pivotal role in accelerating the development and achievements of science and technology in AMO, and in fulfilling shared educational goals. This should be strongly encouraged to continue. Obtaining more than anecdotal data to understand existing interconnections between agencies, with industry, and internationally proved to be especially difficult, so the committee had to draw primarily on our collective experience rather than hard data.

The timing of this AMO decadal survey overlaps well with the increasing effort on QIST as outlined in the recent National Research Council report on the NQI. An entire chapter (Chapter 4) is devoted to addressing this important topic, and the committee emphasizes that AMO continues to play a pivotal role for QIST. Not only does AMO help tackle some of the most fundamental questions related to quantum state engineering, entanglement generation and measurement, and controlled scaling of the number of qubits, but AMO also provides key enabling technologies and some of the most promising platforms that are critical for QIS. In light of the strong national interest in QIST, as seen by the strong support for the NQI, it is clear that AMO will continue to receive a broad base of support for both basic science and emerging technologies, and will play a vital role in creating new opportunities, making foundational discoveries, and providing key enabling technologies for the progress of QIST.

## MAIN FINDINGS AND RECOMMENDATIONS

The committee offers the following findings and recommendations on the AMO scientific front and on government support for AMO. The committee supports each recommendation with a set of findings that the committee has made during the course of this study. These recommendations can be taken to strengthen our responses to specific grand challenges and to broadly advance the entire scientific frontier of AMO.

> **Finding:** The historical strength of AMO has been in its core curiosity-driven AMO research programs, which have been the driving force behind many new scientific discoveries and innovative technologies, including the recent emergence of quantum technology.

**Key Recommendation: It is vital that the U.S. government see curiosity-driven atomic, molecular, and optical science as a critical investment in our economic and national security interests and vigorously continue that investment to enable exploration of a diverse set of scientific ideas and approaches.**

**Finding:** The development of QIST is progressing rapidly, and, while the time is ripe to invest in quantum technology based on specific existing platforms, there is also a large and growing number of possible new systems and platforms one can exploit for construction of quantum machines.

**Finding:** The development of quantum technology is still at a very early stage, and the state of the art is evolving very rapidly. It is too soon to develop governmental standards; however, for the health of the field, the committee finds it is urgent for the research community to develop platform-independent metrics to measure quantum advantage and to characterize the true scientific impact of quantum advantage.

**Key Recommendation: Basic research in science, engineering, and applications underlying both existing and emerging new platforms needs to be broadly supported, including research on techniques for cross-verification of quantum machines across different platforms for various applications. Specifically, the committee recommends that the National Science Foundation, Department of Energy, National Institute of Standards and Technology, and Department of Defense should provide coordinated support for scientific development, engineering, and early applications of AMO-based quantum information systems.**

**Finding:** Creative science carried out by single principal investigator (PI) groups is the heart of AMO science. The field does best building on these individual investigators, but it is entering a new phase where collaborations with flexible-size teams would enable exciting new discoveries.

**Finding:** The development of quantum technology is bringing new opportunities in sensing and precision measurement. However, nurturing these opportunities that impact other areas of science requires long-term investments that cross traditional disciplinary boundaries.

**Finding:** In particular, rapid advances in the precision and capabilities of AMO technologies have dramatically increased the potential of AMO-based techniques to discover new physics beyond the Standard Model. The present lack of a federal funding program dedicated specifically to supporting such research at the intersection of high-energy physics and AMO is a limiting factor in fully utilizing the plethora of opportunities for new discoveries.

**Key Recommendation: The Department of Energy's High-Energy Physics, Nuclear Physics, and Basic Energy Sciences programs should fund research on quantum sensing and pursue beyond-the-Standard-Model fundamental physics questions through AMO-based projects.**

**Finding:** AMO tools, techniques, and data enable the observation and in-depth understanding of a variety of astrophysical phenomena.

**Finding:** State-of-the-art astrophysical observations have identified the need for further development in theoretical and experimental AMO physics, which can help provide in-depth understanding of the cosmos. Addressing these opportunities would require strong interagency coordination that supports AMO and astrophysics.

**Finding:** The time is ripe for recently developed AMO tools and technologies to be deployed in space missions.

**Key Recommendation: The National Aeronautics and Space Administration, in coordination with other federal agencies, should increase investments in theory and experiment for both space- and laboratory-based fundamental atomic, molecular, and optical science that are needed to address key questions in astronomy, astrophysics, and cosmology.**

**Finding:** AMO tools in attosecond and X-ray science are being used to explore a broad range of interdisciplinary topics having implications in chemistry, materials science, and technology. The U.S. position in terms of investment and commercialization in this area has weakened compared to Europe and Asia.

**Finding:** The 2018 National Academies of Sciences, Engineering, and Medicine report *Opportunities in Intense Ultrafast Lasers: Reaching for the Brightest Light* recommended that DOE lead the development of a comprehensive interagency strategy for high-intensity lasers that includes the development and operation of both large-scale national laboratory projects and mid-scale university-hosted projects.

**Key Recommendation: U.S. federal agencies should invest in a broad range of science that takes advantage of ultrafast X-ray light source facilities, while**

**maintaining a strong single principal investigator funding model. This includes the establishment of open user facilities in mid-scale university-hosted settings.**

**Finding:** Experimental AMO science has become very expensive, and making the down payment to start up a new experimental program has become a deterrent for young AMO scientists being appointed as faculty in academia.

**Finding:** Strong theory-experimental collaboration has been important for maintaining the health of AMO science. However, the number of faculty positions in AMO theory has been limited.

**Finding:** There are existing successful portable funding models in the United States and Europe, such as National Institutes of Health (NIH)-K99, and European Research Council grants, that could be used as models to assist faculty appointment and early career development. However, an aspect of the NIH-K99 that would not be appropriate for the U.S. academic physical science community is the level of research effort requirement that makes it incompatible with standard teaching expectations.

**Finding:** Departmental boundaries create barriers for young AMO-trained post-docs to move into related disciplines and departments, such as QIS, computer science, and electrical and mechanical engineering, where their AMO training could play key roles in advancing those fields.

**Key Recommendation: AMO funding agencies should develop portable fellowship grant models that support the transition of AMO science theorists and experimentalists into faculty positions.**

**Finding:** AMO science, like other physics disciplines, continues to have difficulty in attracting women and underrepresented minorities at all levels.

**Finding:** It is clear that education and workforce development in AMO is not keeping up with the demographic shifts in the nation, and that this is a lost opportunity.

**Key Recommendation: The entire AMO science enterprise should find ways to tap into the growing national talent pool of women and underrepresented minorities. The committee therefore endorses the relevant recommendations in the National Academies of Sciences, Engineering, and Medicine**

**report *Graduate STEM Education for the 21st Century* and *Expanding Underrepresented Minority Participation*, for example.**

**Finding:** Quantum technology cuts across scientific fields and technologies beyond AMO, and so encounters barriers with traditional funding mechanisms.

**Finding:** Recent Quantum Leap Initiatives at NSF are based on a stewardship model that starts to break the traditional discipline barriers.

**Finding:** Traditional AMO training focuses on physics; however, the development of quantum technology requires reaching across both academic disciplines and industry to leverage the impact of AMO.

**Finding:** AMO technologies are not being transferred into other fields for use as rapidly as AMO science itself develops. It is increasingly important to let other fields become aware of AMO. The breakneck pace of AMO leads the committee to believe that other communities would benefit from knowing more about AMO.

**Key Recommendation: The National Science Foundation, Department of Energy, National Institute of Standards and Technology, and Department of Defense should increase opportunities for translating atomic, molecular, and optical science advances to other fields by fostering collaboration with scientists and engineers from other disciplines through, for example, support of workshops and similar mechanisms for cross-disciplinary interactions.**

**Key Recommendation: To maximize the effectiveness of federal investment, academia should enable and encourage cross-disciplinary hiring of theorists and experimentalists at the rapidly growing interface between AMO science fields and computer science, mathematics, chemistry, biology, engineering, as well as hiring into industry.**

**Finding:** The health of AMO science relies heavily on strong international collaborations. However, there exist a number of technical and regulatory impediments, including major differences in effort certification, intellectual property ownership policies and conflict-of-interest rules, as well as unfunded external audit requirements and unreasonable currency exchange requirements, all of which make it difficult for U.S. universities to accept and administer grants from, for example, the European Union. While the committee recognizes the significance of potential national security issues, there is great national benefit in having intellectual leaders visiting the United States. This benefit is at risk due to continuing significant issues affecting access to national research facilities and excessive visa delays for international students, collaborators, and speakers at conferences.

**Finding:** Mechanisms for co-funding research that is carried out with international collaboration fuels collective progress in AMO science.

**Key Recommendation: The committee recognizes the real security concerns in open, international collaboration. However, because open collaborations have been so vital for the health of atomic, molecular, and optical physics, the Office of Science and Technology Policy and federal funding agencies should work collaboratively with the Department of State and an academic consortium such as the Council on Governmental Relations to remove impediments to international cooperation. There is a critical need for**

1. **Blanket agreements for funding agencies in different countries to accept each other's grant administration regulations;**
2. **Standardized mechanisms for joint funding of cooperative projects; and**
3. **Mechanisms to remove excessive visa application delays for international students, collaborators, and speakers at U.S. conferences and workshops.**

## CHAPTER-LEVEL FINDINGS AND RECOMMENDATIONS

### Chapter 2: Tools Made of Light

**Finding:** The past decade has seen revolutionary advancements in ultrafast light source development spanning the XUV and X-ray spectral regime. The ability to control and manipulate these tools made of light is enabling new applications that extend beyond AMO physics. New platforms are emerging in QIS, remote sensing, and clocking ultrafast electron dynamics in all phases of matter. Thus, the frontiers lie at the interdisciplinary intersection of physics, engineering, chemistry, materials science, and biology.

**Finding:** Advances in ultrafast X-ray science has become increasingly demanding of resources that are beyond the ability of single PI funding models. X-ray free-electron lasers are large-scale facilities that need the management infrastructure of a National Laboratory. However, table-top systems, such as attosecond- and petawatt-class lasers, have evolved to the level of a mid-scale facility requiring operational management and safety infrastructure. The

United States has lagged behind the rest of the world in capitalizing on the opportunities enabled by these mid-scale facilities, training of a workforce at the cutting edge of technology, and the economic benefits of industrial growth.

**Key Recommendation: U.S. federal agencies should invest in a broad range of science that takes advantage of ultrafast X-ray light source facilities, while maintaining a strong single principal investigator funding model. This includes the establishment of user facilities in mid-scale university-hosted settings.**

**Finding:** Despite the enormous advances of integrated linear and nonlinear photonics based on silicon, there is a need for ultra-low-loss platforms where light can be generated with ultrahigh efficiency, switched and detected, especially for quantum-related applications. Such a platform would probably be formed via the integration of multiple materials on silicon.

**Finding:** Systems exhibiting strong photon-photon interactions are currently being explored, to enable unique applications such as quantum-by-quantum control of light fields, single-photon switches and transistors, all-optical deterministic quantum logic, the realization of quantum networks for long-distance quantum communication, and the exploration of novel strongly correlated states of light and matter.

**Finding:** As nanofabrication technologies and the availability of high optical quality, low thermal dissipation materials improve, design and control of the mechanical oscillators will get more sophisticated. The lower thermal noise of future oscillators will allow quantum fluctuations to fully dominate the motion of the mechanical oscillators, perhaps even at room temperature, creating a versatile quantum resource for a variety of applications.

**Key Recommendation: The federal government should provide funding opportunities for both basic and applied research that enables the development of industrial platforms, such as foundry offerings, and interdisciplinary academic laboratories to support the integration of photonics and engineered quantum matter.**

### Chapter 3: Emerging Phenomena from Few- to Many-Body Systems

**Finding:** Few-body physics continues to be of continuing interest to identify and test the scope of quantum universality, for its intrinsic intellectual interest, its connections with many-body physics, and to strengthen the controllability of both few-body and many-body quantum systems. Developing theoretical tools able to quantitatively predict the behavior and interactions of increasingly complex atoms and molecules is crucial for further developments in these areas.

**Finding:** Due to recent theoretical and experimental breakthroughs, ultracold molecules now constitute a very promising research platform able to tackle diverse many-body phenomena and explorations of fundamental reactive processes, with certain molecules yielding viable targets for precision measurement science.

**Finding:** Trapped ion systems, neutral atoms, systems with long-range interactions (such as those based on molecules and Rydberg atoms) and ion-neutral hybrid systems are leading candidates for quantum information processing and simulation, and for studying chemical dynamical processes.

**Recommendation: The AMO science community should aggressively pursue, and federal agencies should support, the development of enhanced control of cold atoms and molecules, which is the foundational work for future advances in quantum information processing, precision measurement, and many-body physics.**

**Finding:** Quantum gases of atoms and molecules enable controlled exploration of equilibrium and non-equilibrium many-body physics and the generation and manipulation of entangled states applicable to quantum information processing and quantum metrology, and further developing our understanding of deep questions such as the nature of thermalization, many-body localization, and stable quantum matter away from equilibrium.

**Recommendation: Federal funding agencies should initiate new programs to support interdisciplinary research on both highly correlated equilibrium phases and non-equilibrium many-body systems and novel applications.**

**Finding:** AMO-based quantum simulators have the ability in the short term to demonstrate genuine quantum advantage over classical computational devices, without requiring the mastery of complex quantum gates required for a universal digital quantum computer. These systems can provide unique insights into complex models from condensed-matter and high-energy physics, and lead to development and testing of useful quantum algorithms.

**Recommendation: Federal funding agencies should initiate new programs involving development, engineering, and deploying the most advanced**

**programmable quantum simulator platforms, and make these systems accessible to the broader community of scientists and engineers.**

### Chapter 4: Foundations of Quantum Information Science and Technology

**Finding:** There are many possible systems and platforms for construction of quantum machines. The technology development is still at a very early stage and the state of the art is evolving very rapidly.

**Finding:** The federal government has decided to pursue a "science first" policy for QIS.

**Recommendation: In support of the National Quantum Initiative, federal funding agencies should broadly support the basic research underlying quantum information science.**

**Recommendation: Academia and industry should work together to enable, support, and integrate cutting-edge basic research, complemented by focused engineering efforts for the most advanced quantum information science platforms.**

**Recommendation: The Department of Energy and other federal agencies should encourage medium-scale collaborations in quantum information science among academia, national laboratories, and industry.**

**Finding:** The Department of Defense has a long history of supporting AMO research as part of its mission. This has been richly rewarded by numerous developments including the laser, GPS, optics, and a multitude of sensors. More recently, NIST and NSF have joined with DoD, leading to the emergence and nurturing of all aspects of QIS. Most recently, DOE is expected to play a major role in NQI.

**Recommendation: (a) The Department of Defense (DoD) should continue both this foundational support for novel developments and the exploitation of the resulting technologies. (b) U.S. funding agencies participating in the National Quantum Initiative (NQI) should collaborate with each other and with DoD to build on the long history in quantum information science when developing their plans under NQI. (c) Department of Energy and its laboratories should develop strong collaborations with leading academic institutions and other U.S. funding agencies to realize the full potential of QIS.**

### Chapter 5: Harnessing Quantum Dynamics in the Time and Frequency Domains

**Finding:** This is a unique time in ultrafast science due to the ubiquity and controllability of ultrafast light sources spanning the terahertz through the hard X-ray regime. The development and application of these sources have driven much of the progress described in this chapter.

**Finding:** Control of ultrafast electron dynamics in molecular and condensed-phase systems has significant potential for impact well beyond AMO science, including at the technological and industrial levels. Likewise, continued development of molecular movies will drive advances at the fundamental level, and promises societal benefits through improved understanding of photo-driven biological processes.

**Finding:** Continued progress on these challenges will require the combined expertise of multiple PIs and mid-scale infrastructure, either because they involve advanced facilities with many different elements, or because they are inherently multidisciplinary in nature, covering AMO, condensed-matter physics, chemistry, laser technology, and large-scale computation. Funding mechanisms similar to the Physics Frontiers Centers or Multidisciplinary University Research Initiatives, in which multiple PIs from experiment and theory work toward a common goal, are crucial.

**Key Recommendation: U.S. federal agencies should invest in a broad range of science that takes advantage of ultrafast X-ray light source facilities, while maintaining a strong single principal investigator funding model. This includes the establishment of open user facilities in mid-scale university-hosted settings.**

**Finding:** There has been widespread use of data typically gathered in collision physics and spectroscopy, which are needed for applications and analysis in astrophysics, plasma physics, and nuclear medicine among others, as well as a decline in university-supported collision physics and spectroscopy groups.

**Recommendation: National laboratories and NASA should secure the continuation of collision physics and spectroscopy expertise in their research portfolios.**

### Chapter 6: Precision Frontier and Fundamental Nature of the Universe

**Finding:** Rapid advances in the precision and capabilities of AMO technologies have dramatically increased the potential of AMO-based techniques to discover new physics beyond the Standard Model. The present lack of a federal funding program dedicated specifically to supporting such research at the intersection of high-energy physics and AMO is a limiting factor in fully utilizing the plethora of opportunities for new discoveries.

**Finding:** Supporting and promoting much stronger joint efforts between AMO physics, particle physics, gravitational physics, astrophysics, and cosmology is necessary to promote creative ideas and new opportunities for grand challenge discoveries with AMO-based science.

**Finding:** The United States is falling behind in deploying a diverse set of AMO precision measurement platforms and integrating tools into dedicated devices to maximize discovery potential.

**Finding:** International collaborations are needed for full realization of AMO-based science discovery potential.

**Key Recommendation: The Department of Energy's High-Energy Physics, Nuclear Physics, and Basic Energy Sciences programs should fund research on quantum sensing and pursue beyond-the-Standard-Model fundamental physics questions through AMO science-based projects.**

**Recommendation: Federal funding agencies should modify funding structures to allow for theoretical and experimental collaborations aimed at AMO science-based searches for new physics and development of diverse set of AMO precision measurement platforms including larger (more than five principal investigators) and long-term (10-year) projects.**

**Recommendation: Funding agencies should establish funding structures for continued support for collaborative efforts of AMO theory and experiment with particle physics and other fields, including joint projects, joint summer schools, dedicated annual conferences, and so on.**

**Recommendation: U.S. federal agencies should establish mechanisms to co-fund international collaborations in precision searches for new physics with other worldwide funding agencies.**

### Chapter 7: Broader Impact of AMO Science

**Finding:** Other scientific fields, such as the life sciences, have tremendously benefited from AMO science and its tools, as highlighted by single-molecule fluorescence microscopy and adaptive optics being used for super-resolution cellular imaging in near-native conditions. Subsequent advances in synthetic chemistry and materials science have dramatically improved the reach and impact of AMO science and its tools going beyond traditional AMO sciences. Yet, the cross-fertilization between AMO and other fields is not yet occurring at the highest speed possible because of lack of outreach in terms of awareness and availability of the new tools, techniques, and technologies.

**Recommendation: Federal agencies should improve the availability and raise the awareness of the latest AMO technologies for researchers in other fields of science. Additionally, agencies should create funding opportunities to bridge the latest AMO technologies to other disciplines, specifically targeting early adopters.**

**Finding:** Economic development results from AMO-related science and engineering. As exemplified by the University of Rochester, the University of Iowa, the University of Central Florida, the University of Arizona, and Montana State University, state-sponsored centers of excellence in AMO-inspired fields bring researchers and students together from different disciplines in universities, allowing state governments to make connections with industry and thereby promote workforce development. Students at universities benefit from direct exposure to a broader perspective for their coursework selections by direct exposure to what is needed for a career in research and development in industry. This also promotes interdisciplinary research at universities and enhances opportunities for external fundraising for faculty launching new interdisciplinary initiatives.

**Recommendation: State governments should encourage the exploitation of opportunities to compete for economic development in AMO-related science and engineering user facilities at universities using state funding and/or industrial joint support.**

**Finding:** The discussions of engineered quantum matter in Chapters 2 and 4 describe an important emerging field that brings together several disciplines of AMO physics to substantially increase the interaction between material and electromagnetic quantum states. There is great potential for a collaboration between scientists and industry on translational technologies that could miniaturize and scale up a wide range of laboratory-based quantum sensors, including optical clocks and frequency combs. This advance will require a significant increase in the availability of modern advanced photolithography for nanophotonic structures in Si and III-V materials. In addition, students in AMO would benefit greatly from centers dedicated to doctoral training in quantum technologies, modeled on the Centres for Doctoral Training funded by the Engineering and Physical Sciences Research Council in the United Kingdom.

**Recommendation: The National Science Foundation and Defense Advanced Research Projects Agency should create funding opportunities that target strong multidisciplinary collaboration between academia and industry to transfer current e-beam lithography methods in engineered quantum matter to advanced photolithography pilot lines.**

**Recommendation: The National Science Foundation Research Trainee Program should be expanded to ensure that the next generation of post-doctoral fellows are prepared to handle research and innovation challenges across the engineering and physical sciences landscape, particularly in quantum engineering.**

**Recommendation: The federal government should provide funding opportunities for basic research that enable the development of industrial platforms, such as foundry offerings, to support the integration of photonics and engineered quantum matter.**

**Finding:** Astronomical observations have exposed significant shortcomings in our understanding of AMO science that will require significant scientific advances to address. In order to maximize the benefits of ground-based and satellite-based observations, new contributions from AMO theory and experiment are needed to classify the species observed and to understand in detail the elementary atomic and molecular processes occurring in astrophysical environments.

**Recommendation: The National Science Foundation, Department of Energy, and National Aeronautics and Space Administration should support a strengthened community of faculty with the capability to carry out laboratory-based experiments, to develop theory, and to carry out computations in order to maximize the payoff from astrophysical observations and to encourage enhanced support from other funding agencies.**

### Chapter 8: AMO Science: Part of the U.S. Economic and Societal Ecosystem

**Finding:** Funding trends for AMO sciences show, after correction for inflation, little to no increase over the past decade, even as the number of AMO scientists in the United States has grown.

**Key Recommendation: The U.S. government should vigorously continue investment in curiosity-driven AMO science to enable exploration of a diverse set of scientific ideas and approaches. AMO is a critical investment in our economic and national security interests.**

**Finding:** As AMO laboratory programs grow more expensive to seed, the need for seeding the research of early career investigators is increasingly important.

**Recommendation: The federal government should develop seed funding and portable fellowship grant models that support the transition of atomic, molecular, and optical theorists and experimentalists into faculty positions.**

**Finding:** The number of theoretical AMO faculty positions in the United States is perennially low (dangerously low in certain subfields of AMO). AMO theory is an important component of AMO science and presents U.S. scientists with an opportunity to contribute to a vibrant and exciting field.

**Recommendation: A vibrant theory program needs to be incentivized through funding opportunities, such as a portable fellowship grant program, and through a sustained campaign of educating and hiring theoretical AMO physicists.**

**Finding:** The participation of women in AMO science is alarmingly low, with a large gap (relative to white males) in education and career advancement opportunities and outcomes. Systemic barriers to larger participation include societal and institutional biases toward these groups—often unintentional but nonetheless impactful—that lead to already small numbers declining at each career stage. The cultural norms and practices are seen as creating unwelcoming workplaces for these groups.

**Recommendation: Institutions receiving federal funding should implement stronger mechanisms to ensure a high standard of accountability in creating an inclusive workplace environment. Funding agencies may seek ways to incentivize this as well.**

**Finding:** There is little data on underrepresented minorities, but from what we do have, it is clear that the numbers are even lower. The committee has requested data on representation of underrepresented minorities in federal funding and professional society membership, but very little information is available, in keeping with the very low numbers involved. Without high-quality demographic data, the underrepresentation of certain groups continues to be relegated to guesstimation and conjecture. What we do know is that a tremendous opportunity to engage large swaths of American society in AMO science—and in all science, technology, engineering, and mathematics fields—is being squandered. The fraction of scientists in AMO from underrepresented minorities (URMs) is dramatically smaller than the fraction in the general public, making it clear that those benefiting from education and funding opportunities in AMO do not reflect the demographic shifts in the nation, and that is a lost opportunity for the entire field.

**Recommendation: The entire AMO science enterprise should find a multitude of ways to tap into this growing talent pool.**

# 2

# Tools Made of Light

The study of light plays a central role in understanding nature. Light from distant stars reveals the mysteries of the universe and served as a means for humans to circumnavigate the globe. Researchers knew about the existence of a strange form of light dating to the 18th century, but it took the 1895 discovery by Wilhelm Röntgen to identify and harness the light now called X rays. For his discovery's impact on society, Röntgen won the first Nobel Prize in Physics in 1901. Scientists soon recognized that light comes in all different colors, the visible light from stars and Röntgen's X rays were one and the same phenomenon, electromagnetic waves that travel with the same speed in a vacuum. In the 19th century, researchers discovered that gases in a plasma or a flame not only emit the characteristic light we see but also do so in discrete colors. These observations presented a paradox that eluded the mechanics of Newton and stimulated the birth of quantum mechanics in the early part of the 20th century. The expansion of spectroscopy—breaking up light into its component colors—across the electromagnetic spectrum, from X rays to radio frequencies, revealed the quantum structure of matter and unveiled the secrets of the universe.

In 1960, the first demonstration of the laser by Theodore Maiman defined a transformational moment not only in science and engineering but also for society. What was special about laser light? For one, the light, or photons, acted in a collective manner, the so-called coherence property. Consequently, light can have beam-like directional properties, where its composition approaches a single color, or alternatively it can be packed into a brief burst in time. Similar to the curiosity driven activity launched by Röntgen's discovery, current-day scientists are learning to manipulate and harness the light properties, while extending lasing into the X-ray regime. Over the past decade, these advances have produced exquisite tools for enabling unprecedented applications in conveying quantum information, precision tests of foundational physics, and producing movies of the motion of matter. Just as seeing different colors and intensities of starlight partly revealed the nature of the universe, using detectors based on interfering light has provided new eyes on the universe in the form of gravitational waves. This chapter will expand upon this query: What is so special about light?

## GENERATING LIGHT WITH EXTREME PROPERTIES

Lasers have infiltrated everyday life to such a degree that their presence has become ubiquitous and unnoticed. Lasers are used for scanning barcodes at the grocery store checkout counters, for range finders for surveying, for displaying Blu-Ray discs for our viewing pleasure, and for providing precise tools for surgery. The invention and development of the laser has its origin grounded in fundamental atomic, molecular, and optical (AMO) research. In fact, the relationship between light and its applications has been synergistic: engineering new sources enables new science, while research demands drive the development of novel sources, and this remains a modus operandi. In this section, the committee will describe recent advances in the intensity (brightness), time duration, frequency (color), and coherence (oneness) of laser light.

### Intensity

One measure of light is its intensity, a property defined as the power transferred per unit area. Power is the energy (total number of photons) per unit time. The peak power depends on the temporal bunching of the number of photons. Thus, a fixed number of photons arriving in 1 second will have their peak power increased by a billion-fold if bunched into $10^{-9}$ s (nanosecond). Currently, scientists have achieved peak powers of a few petawatts ($1 \text{ PW} \equiv 10^{15}$ W), equivalent to the combined solar power striking the states of California, Arizona, and Nevada on a sunny day at noon; but this power lasts for only 100 femtoseconds ($10^{-13}$ s), a time quite short compared to 1 second. The intensity depends inversely on the beam area, which is proportional to the square of the radial size perpendicular to the propagation direction. The laser cavity or external optics define the area, which cannot be smaller than the wavelength squared. Focusing a PW-class laser beam to a diameter of one wavelength ($1 \text{ micron} \equiv 10^{-6}$ m) yields an intensity of $10^{23}$ W/cm$^2$, which is approximately the current state of the art. Figure 2.1 shows the growth in intensity or equivalent electron energy as a function of year. In the early days of laser development, several technology advances (Q-switching, mode locking)

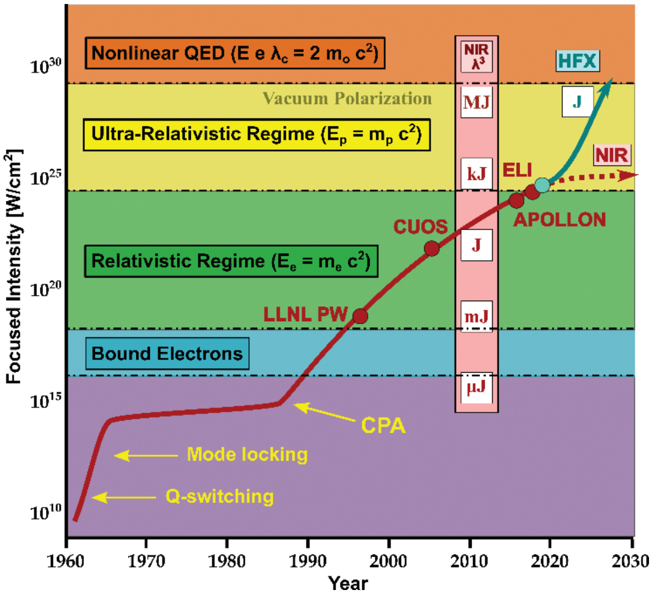

**FIGURE 2.1** The constant progression of laser technology toward higher intensity has allowed exploration of new regimes of light-matter interactions, delineated by the colored regions. In 1986, a seminal moment in laser engineering was the development of the chirped pulse amplification (CPA) architecture, which continues to push the intensity frontier and resulted in U.S. scientists developing the first petawatt laser (LLNL PW—now decommissioned). Several projects are pushing the state-of-the-art over the next several years, but all these efforts are in Europe (ELI, APOLLON) or Asia. However, the scaling of the current near-infrared architecture will saturate in the near future (dashed line labeled as NIR). Beyond this point, new schemes of laser architecture are needed that would be capable of reaching the Schwinger limit of nonlinear quantum electrodynamics (creating matter from vacuum). One high-intensity scheme is indicated by the line labeled HFX, which proposes to generate Joule-level X rays. NOTE: ELI, Extreme Light Infrastructure Project; LLNL, Lawrence Livermore National Laboratory; NIR, near infrared; PW, petawatt; QED, quantum electrodynamics. SOURCE: Courtesy of Dr. Jonathan Wheeler and Dr. Gerard Mourou.

pushed intensity to a limit where the light caused catastrophic material damage thus clamping further gains as illustrated by the intensity plateau near 1970. In 1986, Mourou and Strickland circumvented this problem by the revolutionary technological concept of chirped pulse amplification (CPA; see Figure 2.2), for which they were awarded the 2018 Nobel Prize in Physics. Since that discovery, the intensity has rapidly risen in an analogous fashion to Moore's law for computer chips. This advance resulted in scaling down the highest intensity lasers from facilities operation to table-top systems, thus opening numerous opportunities in AMO and plasma physics. CPA lasers producing intensities equivalent to the atomic field (regime of equivalent field strength as an electron bound to a proton in the hydrogen atom) enabled the rapid progress in ultrafast and extreme nonlinear science

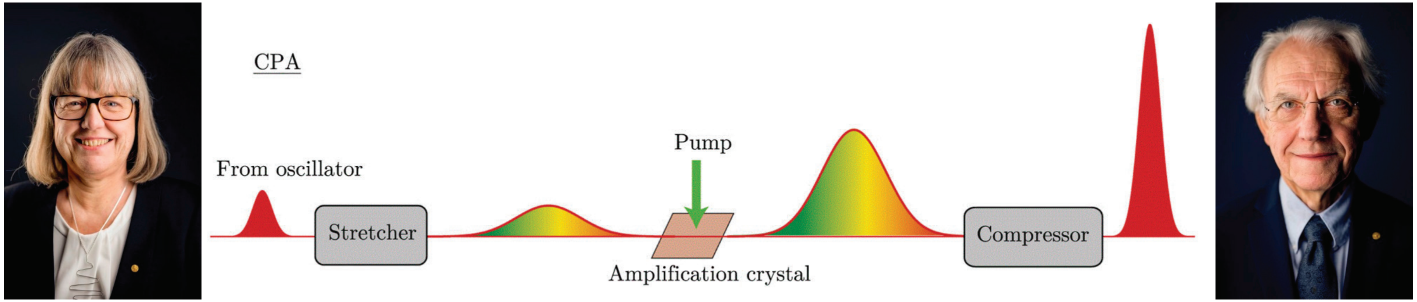

**FIGURE 2.2** Chirped pulse amplification (CPA) revolutionized high-intensity, ultrafast laser technology. Part of the 2018 Nobel Prize in Physics was awarded to Donna Strickland (left) and Gerard Mourou (right) for the discovery of CPA. Prior to this seminal work, material damage limited high-intensity amplification of short pulses. CPA circumvented this problem by first temporally stretching a weak femtosecond pulse by several orders of magnitude by introducing a group velocity dispersion (GVD). The consequence is an equal reduction in the peak power. The stretched chirped pulse is then amplified in a suitable laser gain medium to near damage threshold—that is, in this example a 106-109 times in pulse energy. Last, a pair of gratings configured to introduce a positive GVD compresses the amplified pulse close to the original femtosecond pulse duration. SOURCE: The central graph is from the CELIA website, http://www.celia.u-bordeaux1.fr/spip.php?article254&lang=fr. The portraits are from the Nobel Foundation.

discussed in Chapter 5. At the current state-of-the-art intensities ($10^{23}$ W/cm$^2$), electrons become highly relativistic—that is, their motion approaches the speed of light, and must be described by physics beyond Maxwell's equations. In addition, these high intensities are enabling the production of secondary particles (X rays, protons, neutrons) emerging from gas and solid plasmas that are finding applications in national security, astrophysics and cancer therapy.

Several ongoing frontier efforts in Europe, Korea, China, and Japan based on CPA are pushing the technology to new limits. Most notable is the Extreme Light Infrastructure (ELI) project of the European Union. The ELIs are composed of three pillars located in Hungary, Czech Republic, and Romania. These facilities will push the intensity by 100-fold, enabling the exploration of light-driven particle acceleration, nuclear physics, and zeptosecond ($10^{-21}$ s) pulses. Clearly, Europe and Asia have taken leadership in a technology pioneered in the United States. The consequence of this has been a steady decay of technical competency and industrial innovation in the United States.

As shown in Figure 2.1, current CPA projects are all based on increasing the power by scaling the geometric growth of the amplifiers, which will ultimately plateau (see dashed line) similar to the earlier period before CPA. To push beyond this limit, novel optical architectures need to be developed. One approach under discussion is the "lambda-cubed shortcut." The idea is to increase the intensity by decreasing the beam's area and duration through shortening the wavelength.

Another transformative event occurred in fall 2009 with the operation of the world's first X-ray free-electron laser (XFEL) at SLAC National Laboratory. The FEL concept is distinct from optical lasers for several reasons, but one major difference is that the lasing medium is not a physical material—for example, a crystal, or a diode—but a relativistic beam of electrons. In the 1970s, researchers developed FEL devices lasing in the mid-infrared/ultraviolet regime using optical resonators inserted into straight sections of a circular electron storage ring. However, operation was limited to the optical regime due to a combination of poor gain and low reflectivity of optics. Consequently, interest in FEL technology declined because these devices could not compete with traditional lasers. In the 1990s, a revolutionary approach emerged based on high-gain, single-pass lasing, which eliminated the need for resonator optics but at the cost of linear electron accelerators with high peak current. At first light, the Linac Coherent Light Source (LCLS) at SLAC performance at 1.5 Angstrom exceeded the peak spectral brilliance of all previous X-ray sources by more than a billion-fold. Truly revolutionary! The X rays had millijoule (mJ) energy, an attribute common to optical lasers but unprecedented from X-ray sources. Figure 2.3 presents a brief tutorial on the XFEL principle.

Another advance closely related to intensity is the repetition rate for delivering the light pulses. In an experiment, the real time to accumulate a signal is a

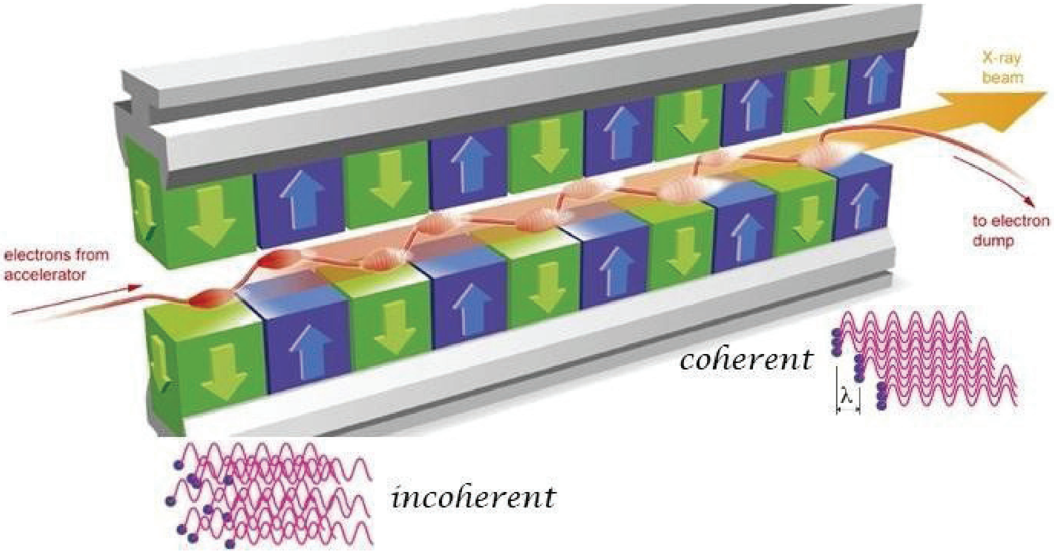

**FIGURE 2.3** The majority of current X-ray free-electron lasers (XFEL) operate on a principle known as Self Amplified Stimulated Emission (SASE). A pulse of relativistic electrons traveling in a straight line at nearly the speed of light propagates into a periodic magnetic structure with alternating north-south poles known as an undulator. Upon entering, the electrons experience a magnetic force and undergo an oscillatory motion as they propagate down the undulator. When properly phased, the oscillating electrons radiate light. Initially, each electron in the pulse radiates independently such that the light fields are incoherent. However, through the SASE process the electrons progressively micro-bunch together at a wavelength commensurate with X-ray emission. At this point, the electrons radiate in concert and the number of X-ray photons increases exponentially. The coherent process continues to emit more and more X rays as the micro-bunch propagates down the undulator. Last, at the end of the undulator saturation terminates the gain. The emerging X rays travel in a straight line to perform experiments while a magnetic field deflects the electron pulse into the ground. This sequence is repeated for subsequent electron pulses at repetition rates that vary from 0.01-1,000 kHz depending on the XFEL design. XFELs are transforming the landscape of X-ray science, enabling the structural determination of macromolecules relevant to life and providing an unprecedented tool for producing molecular movies (see Chapter 5). SOURCE: Modified from European XFEL webpage, https://www.xfel.eu/facility/overview/index_eng.html.

critical element in evaluating the feasibility for performing a measurement. Thus, the average power, defined as the total energy delivered over 1 second, is another critical experimental parameter. A standard commercial table-top CPA laser system operating in the near-infrared (NIR) produces 1-25 W of average power at repetition rates spanning 0.1 to 1 kHz. However, there has been a dramatic change in the average power capabilities of table-top lasers. The state-of-the-art table-top lasers are operating at kilowatt average power at 0.1 to 1 MHz repetition rates. These advances, which are mainly occurring in Europe, are rapidly moving onto the commercial market. The challenges associated with thermal management are being circumvented by new methods based on coherent combination of fiber amplifiers outputs or optical parametric amplifiers. Likewise, in the X-ray regime, the next generation of XFEL coming online will also move performance from the 120 Hz of the initial LCLS project into the megahertz regime for the European XFEL and LCLS II in the United States. In these cases, the enabling technology is superconducting electron accelerators, which will push the average power to 200 W level.

Each of these advances enables more precise experiments and greater user access while transforming our understanding of light-matter interactions. AMO scientists play a central role in the technology and science. Some of the science enabled by these parameters are highlighted in Chapter 5.

## Time

As illustrated in Figure 2.4, scientists are faced with the daunting task of clocking natural phenomena over a broad range of time scales. Over the past decade, the emergence of new transformational tools has expanded the time scales to include the clocking at the molecular and electronic levels.

The duration of a light pulse has far-reaching consequences beyond defining its power. The uncertainty principle dictates a strict inverse relationship between frequency and time. The shorter the time duration of a pulse, the larger the uncertainty in its frequency content, or conversely, a laser with a well-defined frequency

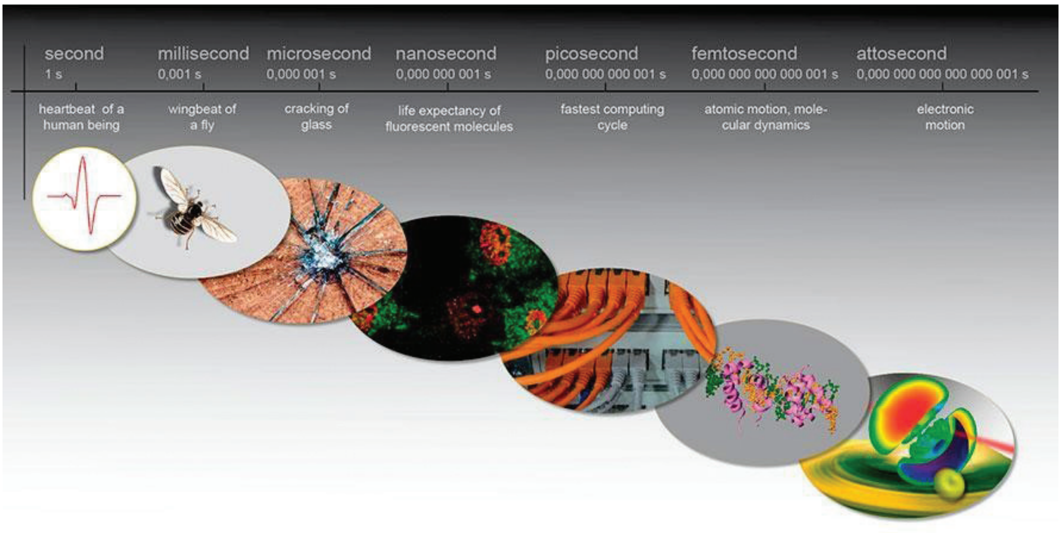

**FIGURE 2.4** Natural phenomena cover a broad range of time scales. Using the human experience as a reference point, AMO scientists employing ultrafast laser pulses have pushed the precision of time to unprecedented limits. In fact, the attosecond scale is as absurdly small a slice of time as the age of the universe is unimaginably long ($10^{18}$ s). SOURCE: Courtesy of Thorsten Naeser.

requires a long coherence time. The committee defers discussion of ultra-narrow laser operation for the next section. Instead, here it will examine time in the context of producing a "movie" of matter on specific physical or chemical time scales. A movie represents a series of snapshots that, when played back in sequence, reveals motion. The key is that the "camera shutter" is fast enough to freeze the motion in a single snapshot. For AMO scientists working with ultrafast technology, the "shutter" is the brevity of the light pulse. Figure 2.4 illustrates the time scale of natural and technological processes. The second is a good metric of human experience, the beat of a heart. The beating of a fly's wing is a thousand times faster ($10^{-3}$ s), while phenomena like shock propagation in glass or fast chemical kinetics is even faster ($10^{-6}$ s). The lifetime of a fluorescing molecule or flipping a central processing unit (CPU) bit in a classical computer takes nanoseconds to picoseconds.

Biological movement and chemical kinetics typically happen at times longer than nanoseconds ($1 \text{ ns} \equiv 10^{-9}$ s). Moving to shorter light pulses, one enters the time scale defined by the rotational (picoseconds $\equiv 10^{-12}$ s) and vibrational (femtoseconds $\equiv 10^{-15}$ s) motion of the nuclear constituents of a molecule. Laser pulse technology producing femtosecond durations are ideal probes of this molecular motion; pioneering work resulted in the 1999 Nobel Prize in Chemistry being awarded to the late Professor Ahmed Zewail.

Femtosecond light pulses from lasers remain the routine ultrashort tool to this day, but in 2001 a watershed moment occurred in laboratories in Paris and Vienna, when the first formation of attosecond ($1 \text{ as} \equiv 10^{-18}$ s) light pulses gave birth to the attosecond era, and enabled the study of electron motion in matter on its natural time scale. For example, the orbit time associated with the electron in the ground state of the Bohr atom is 150 as.

CPA technology was crucial for this discovery since attosecond pulse generation results only when an intense laser pulse possessing an atomic unit of field[1] interacts with an atomic sample (the bound electron regime shown earlier in Figure 2.2). This extreme nonlinear interaction leads to the process of high harmonic generation (HHG). In the frequency domain, HHG produces a coherent frequency comb or plateau of odd-order harmonics whose Fourier synthesis in time is a train of attosecond pulses or an isolated attosecond pulse. These tabletop sources can extend into the kilovolt spectral regime, although the majority of applications are performed in the extreme ultraviolet (XUV) to soft X-ray regime. Current state-of-the-art HHG sources have produced attosecond pulses with durations of two atomic units of time ($1 \text{ au} \equiv 24.2$ as).

In the future, high-intensity relativistic interactions resulting from a laser interacting with a solid surface could break the attosecond barrier opening the

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[1] The atomic unit of field is defined as the Coulomb field strength between the electron and proton in the ground state of the hydrogen atom and has a value of 50 V/Å.

possibility of zeptosecond bursts ($10^{-21}$ s). In one model, the ionized (plasma) surface oscillates at relativistic speeds producing a Doppler shifted laser light at much higher frequencies: a harmonic comb extending deep into the X-ray regime. In principle, all the frequencies are phase-locked, thus capable of producing not only attosecond but also potentially zeptosecond ($1 \text{ zs} \equiv 10^{-21}$ s) bursts. At this time scale, scientists would be able to time resolve nuclear processes.

XFEL facilities are defining not only the intensity frontier in X-ray science but also a new vista in time. For decades, synchrotron facilities produced periodic burst of X rays of ~100 ps, but XFELs have demonstrated performance down to 1 fs, shortening pulse durations by five orders of magnitude. Furthermore, proof-of-principle experiments have demonstrated that the next-generation XFELs will have operational capabilities on the attosecond time scale.

### Frequency, Bandwidth, and Coherence

The use of light across the electromagnetic spectrum is a foundational tool in modern-day AMO physics covering spectroscopy, cooling, clocks, ultrafast, metrology, and imaging. The color of light is often thought of as defined by its frequency, which is a measure of the number of oscillations of the electromagnetic wave in 1 second, expressed in Hertz ($s^{-1}$) in SI units. In vacuum, the frequency is proportional to the speed of light divided by the wavelength. In the context of science and technology, the electromagnetic frequency spectrum is continuous, extending from radio (kilohertz) to gamma-ray (yottahertz = $10^{24}$ Hz) frequencies. A beam of light, whether a continuous wave or pulsed, is characterized by a carrier or central frequency and a distribution function—for example, bandwidth. Different parts of the frequency spectrum are utilized to probe and control specific aspects of matter. Visible light, detectable by the human eye, occupies a small portion of the electromagnetic spectrum from 0.4 to 0.8 petahertz ($1 \text{ PHz} = 10^{15}$ Hz). In spectroscopic applications, the frequency of the light is relevant for exciting specific quantum transitions in matter. Typical electronic transition frequencies from the ground state to other bound states occur in the visible to the vacuum ultraviolet (6 PHz), while excitation among Rydberg states, fine, and hyperfine structure occur at much lower frequencies. In molecules or solids, the additional degrees of freedom from nuclear movement have transition frequencies covering the microwave (gigahertz) to infrared ($100 \text{ THz} = 10^{12}$ Hz) regions. At frequencies higher than the vacuum ultraviolet, light becomes ionizing, freeing electrons from valence and inner shell states. Determining the molecular structure occurs at hard X-ray frequencies (30 PHz to 20 exahertz), where the wavelength becomes smaller than the atomic distances in matter.

Two important properties that determine the light's spectral content are bandwidth and coherence. The bandwidth is the range of frequencies contained in the light, and the coherence defines the phase relationship between the different colors in space and time. For fully coherent Fourier transform limited light, the bandwidth is simply related the inverse duration. Thus, a two-cycle visible laser pulse has a bandwidth comparable to the carrier frequency, while a highly monochromatic laser requires continuous wave operation. However, the high temporal and spatial coherence of a laser makes it ideal for producing waveforms that span the visible and infrared regions of the spectrum. By harnessing nonlinear optical processes, it is possible to extend laser-like coherence properties over the entire ultraviolet and soft X-ray regions. These qualities are transforming the utility of light in ultraprecise measurement and ultrafast science.

In laser science, the control of optical phases is paramount. In the spectral domain, continuous wave lasers are providing dramatically enhanced resolving power to see ever finer energy structures of matter. Ultrastable lasers that maintain optical phase coherence for tens of seconds make it possible to investigate optical transitions with resolution approaching one part in $10^{16}$. Many new scientific thrusts have emerged from that quest, such as testing for fundamental symmetries, developing sensors of increasing sensitivity, probing the quantum nature of many-body physics, and searching for new physics beyond the standard model. The best atomic clocks are now based on stable light interacting with degenerate quantum matter confined in laser fields. With significant increases in the quality factor of the atomic transition and the improved characterization and control of systematic effects, optical atomic clocks have progressed to an accuracy level of $10^{-18}$, which is two orders of magnitude improved from current standards.

The increased temporal resolution enabled by the combination of ultrafast lasers and extreme nonlinear optics opens the door to probe the fastest electron dynamics that occur on femtosecond to attosecond time scales. A femtosecond mode-locked (ML) laser generates a periodic train of short pulses in time that corresponds to a comb structure in the frequency domain. Thus, phase stabilization techniques can be straightforwardly applied to the pulse train to control both the repetition rate and the optical carrier frequency with respect to the pulse envelope. Equivalently, the broad spectral coverage of the frequency comb provides phase control of optical frequency markers across intervals of many hundreds of terahertz, enabling ultraprecise measurements and coherent spectroscopy that possess both ultrahigh spectral resolution and ultrawide spectral bandwidth.

## MANIPULATING THE PROPERTIES OF LIGHT

The triumph of optical technology in the past decade is not only linked to the advances in generating unique properties of light but equally the ability to precisely manipulate these properties. In essence, the AMO scientist has the ability to sculpt the light into a waveform that can guide the interaction with a quantum system. This section highlights some of these attributes.

## Spectral Manipulation

As discussed above, ultrashort laser pulses are intrinsically broadband. In a method commonly termed pulse shaping, coherent bandwidth from an ML laser can be transformed into nearly arbitrarily shaped, user-defined waveforms. In one commonly used approach, the frequency components are spatially separated, manipulated in parallel in both amplitude and phase, and then put back together into a single beam. Thus, the output waveform is simply the inverse Fourier transform of the spatial pattern transferred onto the complex optical spectrum. Pulse shaping has found widespread applications both in technology and ultrafast optical science. User-defined ultrafast waveforms have been used to explore laser "optimal" control over photochemical reactions and quantum mechanical processes in matter, in implementation of multidimensional optical spectroscopies, in compressing pulses to durations approaching the oscillation period of visible light, and to deliver the shortest possible pulses at the foci of microscope objectives for nonlinear biomedical imaging and laser machining.

One important direction was inspired by the development of optical frequency comb (OFC) lasers. OFC sources highlight the discrete nature of the ML spectrum and provide a stable phase relationship between adjacent pulses in a ML train. This led to the quest for line-by-line shaping, also termed optical arbitrary waveform generation, in which spectral control is exercised independently on individual comb lines, with the consequence that unlike earlier pulse shaping experiments, the shaped field now expands to fill time. A challenge was that ML laser frequency combs generally have line spacing below ~1 GHz, too fine to be resolved by most pulse shapers. For this reason, line-by-line pulse shaping has been performed with new comb sources in which a continuous-wave laser is converted to a coherent broadband pulse field, either via strong electro-optic phase modulation or via nonlinear wave mixing in photonic microresonators (so-called Kerr combs). Such alternative comb sources provide much wider frequency spacings and bring new features such as flexible tuning and implementation in integrated photonics.

In an alternative direction, pulse shaping has impacted quantum optics. Although originally developed for manipulation of coherent ultrashort light pulses, it is equally applicable for spectral phase and amplitude filtering of any broadband optical signal. When applied to broadband time-energy signal and idler photons, generated for example via spontaneous parametric down conversion, it enables programmable reshaping of the time correlation function between the two photons. This operation is mathematically analogous to what occurs in classical ultrafast optics but has a distinct physical interpretation. The most recent works involve manipulation and measurement of quantum states of light in which quantum information is encoded as superpositions of discrete frequency bins—a relatively new degree of freedom for quantum information with photons. Quantum information applications include generation of high-dimensional units such as qudits, which can carry multiple qubits per photon, robust transmission over fiber, frequency parallelism and routing, compatibility with on-chip microresonator sources, and potential for hyperentanglement with other photonic degrees of freedom such as different spatial or angular momentum modes.

### Spatial Manipulation

Recently novel ways to spatially manipulate light have emerged, largely based on ideas drawn from solid-state phenomena. These manipulations open the door for structures that are reconfigurable and enable arbitrary localization and emission of light. Photonic topological insulators, for example, proposed a decade ago by Raghu and Haldane,[2] provide one-way spatial guiding of light that is robust against fabrication imperfections, even around sharp corners and bends. Photonic topological insulators have been experimentally realized in passive structures such as arrays of silicon rings or arrays of helically curved waveguides. Additionally, topological lasers with arbitrary geometries have been demonstrated, where the emission is spatially localized along the one-way edge mode. Photons are neutral particles, and hence there is no naturally existing gauge field that couples to photons. Nevertheless, effective gauge potentials for photons can be created in dynamically modulated photonic structures. In these recent demonstrations, light is spatially localized not by a boundary between a high-index region and a low-index region, but by a boundary between regions with different gauge potentials.[3]

Anderson localization leverages disorder and many-body interactions to strongly localize light by coherent interference from scatterers, in contrast to topological photonics that relies on order and periodicity for spatial guiding. Over the past decade, initial demonstrations of classical Anderson localization have been extended to the quantum regime with entangled photons, which show surprising behavior such as counterintuitive bunching or anti-bunching. Studies have also been carried out for localization and wave propagation in quasicrystals—a class

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[2] S. Raghu and F.D.M. Haldane, Analogs of quantum-Hall-effect edge states in photonic crystals, *Phys. Rev. A* 78:033834, 2008.

[3] For an extensive review of topological photonics and gauge potentials, see T. Ozawa, H.M. Price, A. Amo, N. Goldman, M. Hafezi, L. Lu, M.C. Rechtsman, D. Schuster, J. Simon, O. Zilberberg, and I. Carusotto, Topological photonics, *Rev. Mod. Phys.* 91:015006, 2019.

of structures made from building blocks that are arranged using well-designed patterns but lack translational symmetry.[4]

Metamaterials offer a unique approach for spatial light modulation with a subwavelength resolution. Metamaterials consist of a large number of spatially varying resonators arranged in a subwavelength-scale lattice. One can engineer each resonator almost independently via its geometry to manipulate the amplitude, phase, or polarization of light. This enables extremely large flexibility for full spatial control of the electromagnetic field. For example, metamaterials can realize an aberration-free lens with a high numerical aperture, which produces a strongly convergent wavefront. This complete spatial control of electromagnetic field enables the generation of holograms and structured light beams and the realization of cloaking. One can also exploit the high spatial resolution to multiplex several functionalities in one metamaterial. Metamaterials can be classified by the two types of subwavelength resonators—plasmonic and dielectric resonators. Plasmonic resonators allow deeply subwavelength sizes for extremely high spatial resolution, while suffering from inevitable material absorption from metals. Dielectric resonators, on the other hand, circumvent material absorption by using high-refractive-index dielectric materials such as silicon, silicon nitride, and titanium dioxide. In spite of the lower spatial resolution compared to their plasmonic counterparts, the high efficiency and the potential for Complementary metal–oxide–semiconductor (CMOS)-compatibility of all-dielectric metamaterials have attracted great attention lately. Currently, there is still a lack of effective approaches to tune the large number of resonators dynamically, which will require further research to incorporate tunable materials such as two-dimensional (2D) materials and phase-change materials.

## Quantum Manipulation

The realization of strong interactions between individual light quanta (photons) is a long-standing goal in optical science and engineering that is of both fundamental and technological significance. While it has been known for more than half a century that light fields can interact with each other inside nonlinear optical media, at light powers corresponding to individual photons the nonlinearity of conventional materials is completely negligible. Remarkable advances in quantum optics over the past decade have recently culminated in experimental demonstrations of several methods to generate optical nonlinearities at the level of individual photons.

A long-standing goal in optical science has been the implementation of nonlinear effects at progressively lower light powers or pulse energies. The ultimate

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[4] Z. Vardeny, A. Nahata, and A. Agrawal, Optics of photonic quasicrystals, *Nature Photon* 7:177-187, 2013, https://doi.org/10.1038/nphoton.2012.343.

limit may be termed quantum nonlinear optics, where individual photons interact so strongly with one another that the propagation of light pulses containing one, two, or more photons varies substantially with photon number. While this regime is difficult to reach because of the small nonlinear coefficients of bulk optical materials, the potential payoff is significant. On one hand, the realization of quantum nonlinear optics could improve the performance of classical nonlinear devices, enabling—for example, fast energy-efficient optical transistors that avoid Ohmic heating. On the other hand, nonlinear switches activated by single photons could enable optical quantum information processing and communication, as well as other applications that rely on the generation and manipulation of nonclassical light fields.

Over the past decade, this long-standing goal of quantum nonlinear optics was achieved using the complementary approaches of cavity quantum electrodynamics (cQED) and Rydberg-blockade mediated photon-photon interactions. The cQED approach to enhance the atom-photon interaction probability, beyond what is possible with a tightly focused laser beam, is to make the photon pass through the atom repeatedly. This can be achieved by means of an optical cavity. An optical cavity comprises two (or more) highly reflective mirrors between which the light can bounce multiple times before escaping due to transmission or losses. In this case, the interaction probability is enhanced by the number of bounces the photon makes between the mirrors before leaving the cavity, which is conventionally quantified by the cavity "finesse." Taking the multipass atom-photon interaction into account, one can define a quantity called cooperativity—that is, how close the interaction probability approaches unity—enabling strong nonlinear interactions at the single-photon level. Over the past decade, systems with cooperativity approaching 50 were realized. This approach led to the realization of a single-photon transistor and of a single-photon phase switch as well as quantum logic operations and entanglement of individual photons using the strong coupling of a single trapped atom or a single atom-like color center to the optical cavity. These techniques were already used to realize optically mediated interactions between two color centers in nanophotonic cavity and quantum logical gates between two trapped atoms.[5] They pave the way toward integrated quantum networks involving multiple atomic nodes connected by guided light, as discussed in Chapter 4.

An alternative approach, which does not require optical resonators, makes use of strong atom-atom interactions associated with atomic Rydberg states. Atoms in such states have large orbits resulting in large polarizability and greatly

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[5] R.E. Evans, M.K. Bhaskar, D.D. Sukachev, C.T. Nguyen, A. Sipahigil, M.J. Burek, B. Machielse, et al., Photon-mediated interactions between quantum emitters in a diamond nanocavity, *Science* 362(6415:662-665, 2018, https://doi.org/10.1126/science.aau4691.

enhanced interaction strength. By strongly coupling incoming photons to such states, via, for example, electromagnetically induced transparency, strong long-range dipolar interaction between two Rydberg atoms can mediate a strong effective photon-photon interaction of propagating photons down to the level of individual light quanta. Realization of such systems has been a long-standing goal in nonlinear optics community. With this approach, researchers realized an optical medium that transmits one photon, but absorbs two; a bound state between two and three photons and a robust nonlinear phase shift between two individual photons.

Systems exhibiting strong photon-photon interactions are currently being explored to enable unique applications such as quantum-by-quantum control of photon states, single-photon switches and transistors, all-optical deterministic quantum logic, the realization of quantum networks for long-distance quantum communication, and the exploration of novel strongly correlated states of light and matter. Some of these exciting new developments are discussed in subsequent chapters of this report.

### Squeezed States of Light

Quantum correlations of light extend beyond the single photon regime. Indeed, continuous wave light beams also have quantum descriptions and can be manipulated for applications in sensing and metrology. One such quantum state of light is a squeezed state, which can increase the precision of optical measurements, most notably in laser interferometers. Quantum uncertainty imposes a fundamental limit on the precision with which complementary quantities—for example, position and momentum of a particle—can be simultaneously measured. Squeezed states of light manipulate this limit by decreasing the noise in either the phase (or amplitude), while simultaneously increasing the noise in the orthogonal property—amplitude (or phase)—hence “squeezing” the minimum uncertainty. Thus, a measurement will have greater precision if the detected signal lies in its squeezed state, without contamination from the orthogonal property, which is necessarily much noisier.

The applications of squeezed light include radiometry, quantum sensing, and quantum key distribution. However, one of the great successes is its application to gravitational wave detectors, where squeezed light increases the sensitivity of the optical measurement at the output of the kilometers-long laser interferometers. This is a beautiful example of AMO techniques developed for a revolutionary astrophysics instrument, and is described in greater detail in Chapter 6.

In the near future, as squeezed light sources are engineered to be more portable and integrated, this technology can improve the precision of any quantum-limited optical measurement. Some significant challenges that must be overcome to realize this are lower loss linear and nonlinear optical components, higher efficiency photodetectors, and optical interfaces.

## EMERGING PLATFORMS

Light-based technologies have allowed the development of several "platforms" that may be used for many different applications. In this section, the committee describes a few of these versatile platforms and the advances they have enabled.

### Optical Control of Color Centers in the Solid State

Crystallographic defects, dubbed color centers, particularly in wide-bandgap materials, have become fertile platforms for light-matter coupling, quantum information processing, and quantum sensing. Research on quantum control of atom-like impurities in the solid state aims to bridge the gap between the advantage of well-defined quantum properties present in isolated atoms and the possibility to create conditions for strong interactions and integration into nanoscale solid-state devices by combining the best of both worlds of atomic and condensed-matter qubits. Formed by introducing localized defects, such as low-concentration dopants, in solid crystals, these impurities feature tightly localized orbitals, with electronic states that resemble those of individual atoms. In other words, they behave essentially as single atoms frozen inside a solid lattice. Similar to atoms and ions, quantum mechanical superpositions of their states can be prepared and manipulated using coherent control techniques developed by the AMO physics community. Remarkably, this can sometimes be accomplished using optical techniques even under ambient, room-temperature conditions. Moreover, because of the tight localization of their wave functions, atom-like systems can be strongly coupled to other systems and degrees of freedom, such as nuclear spins in the lattice, photons, or phonons. Recent experiments show that atom-like systems may enable far-reaching control over quantum states, with applications ranging from information processing and quantum communication to biological sensing.

The nitrogen-vacancy (NV) center in diamond is a prototypical example of an atom-like system. This quantum defect is formed by a nitrogen impurity next to a missing carbon, or vacancy, and can be created naturally or by nitrogen ion implantation and annealing. The electrons occupying the dangling bonds around the vacancy play the role of the electrons bound to the nucleus of an atom or ion, exhibiting long-lived spin states and well-defined optical transitions. The electronic states lie deep within the wide indirect bandgap of diamond, and are thereby energetically isolated from the Bloch states of the crystal. Furthermore, the low spin-orbit coupling in diamond, as well as its mostly spinless carbon-12 lattice, create an ideal solid-state environment for spins. Thus, despite the fact that the NV defect is surrounded by nearest-neighbor atoms only angstroms away, its states are so well isolated from environmental perturbations that their coherence properties can be comparable to those of an atom trapped in ultrahigh vacuum. Over the past decade, NV centers have been used to realize long-lived quantum memory and multiqubit quantum registers, realize and probe novel phases of matter away from equilibrium such as discrete time crystals (see Chapter 4), create long-distance entanglement that has been used for first loophole-free violation of Bell inequalities, and realize unique applications for nanoscale sensing. Specifically, magnetometers based on NV centers were able to record nuclear magnetic resonance (NMR) signals from individual molecules and picoliter-scale samples with sufficient sensitivity to perform analytical NMR spectroscopy of single cells (see Chapter 4). These techniques are already being employed for practical applications in biomedical diagnostics.

Moreover, over the past few years many other atom-like defects, both in diamond and other wide-bandgap materials, have been actively explored. Some of them may possess properties that are superior to those of NV centers for certain applications. For example, a silicon-vacancy (SiV) centers in nanophotonic diamond system was used to efficiently generate a coherent optical interface for the generation, storage, entanglement, and manipulation of individual photons. These features, which arise from an inversion symmetry associated with SiV centers, make them an intriguing alternative to NV centers, with potentially superior properties for quantum optics and quantum networking applications For instance, very recently, SiV centers were employed for the first demonstration of memory-enhanced quantum key distribution (see Chapter 4). At the same time, defects in silicon carbide and 2D materials are being actively explored. Identifying and custom-designing atom-like systems with desired properties is an active topic in materials science research.

## Integrated Optics

In the past decade, the photonic community witnessed a complete transformation of optics. Scientists went from being able to miniaturize a handful of devices to being able to define and control the flow of light using thousands of monolithically integrated optical components—all on a silicon chip. The key to enable this massive integration is the decrease of optical loss. In the past decade, propagation losses in waveguides have decreased by orders of magnitude thanks to advances in semiconductor processing. Chip-scale long optical delays (see, for example, Figure 2.5) can now be realized, due to the recent development of photonic platforms that can transmit light confined to submicron-size waveguides, over very long distances with low optical losses.

The field of integrated optics and in particular silicon photonics is rapidly evolving and is now enabling completely new applications, ranging from Lidar to quantum platforms. While the initial drive for silicon photonics in the early 2000s

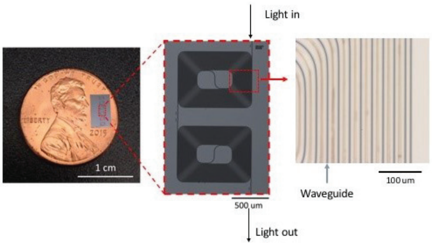

**FIGURE 2.5** A 0.4-meter-long waveguide packed within an 8 $mm^2$ area on a silicon chip. Such chip-scale long optical delays are enabled by the recent development of photonic platforms that can transmit light confined to submicron size waveguides, over very long distances with low optical losses. SOURCE: X. Ji, X. Yao, M. A. Tadayon, A. Mohanty, C. P. Hendon, and M. Lipson, "High Confinement and Low Loss Si3N4 Waveguides for Miniaturizing Optical Coherence Tomography," paper SM3C.4 in Conference on Lasers and Electro-Optics, OSA Technical Digest (online), Optical Society of America, 2017.

was the ability to transmit and manipulate ultrahigh bandwidth with low power dissipation, new applications are continually emerging. This is partly due to the development of novel chip-scale devices and materials compatible with silicon photonics. Many of these technologies and devices can manipulate light across the whole visible, infrared, and mid-infrared spectrum.

For nonlinear optical phenomena that enable the generation and manipulation of light across different spectral domains, chip-based platforms offer several key advantages over bulk and fiber geometries. The first is that most of the photonic-chip materials (e.g., silicon nitride, lithium niobate) have relatively high effective nonlinearities as compared to silica glass. More importantly, a critical property of these materials is the high refractive index contrast between the core waveguide and the cladding layer. For example, materials such as silicon and silicon nitride have refractive indices of 3.4 and 2.0, respectively, at 1.55 µm wavelength, and are typically covered by a silicon oxide cladding layer with an index of 1.46. This large index contrast allows for light to be strongly confined to an area smaller than the wavelength squared, which greatly enhances the effective nonlinearities due to the increase in power, over distances that can be as long as 1 m. This tight confinement also allows for dispersion engineering by tuning slightly the size and shape of the waveguide to phase match optical parametric processes over extremely broad bandwidths.

As an example of the power of integrated optics for nonlinear optics, microresonator Kerr combs have been demonstrated in a variety of platforms, including in a silicon platform that is fully compatible with standard microelectronic processing platforms. Their spectral coverage extends to the visible and mid-infrared, and repetition rates in the microwave regimes have been achieved. More importantly, such chip-scale frequency combs can generate fully coherent optical frequency combs with a bandwidth limited only by dispersion and transparency. Such soliton microcombs have in the past years been applied successfully to ultrafast ranging, astrophysical spectrometer calibration, terabit per second data communication, as well as dual comb spectroscopy.

The area of nonlinear optics in these integrated platforms could enable a technology that is robust enough to be deployed at a large scale, and operate with power levels that are relevant for use in satellites or mobile devices. In a similar vein, optical losses in fibers, on the order of decibels per kilometer (dB/km; 1 dB ~ 25 percent), are more than four orders of magnitude smaller than those in integrated photonics, but little is known about where the latter losses stem from, and how they can be mitigated. This will require innovative approaches beyond the traditional ones employed to date. Likewise, integrated nonlinear photonics can be leveraged with new materials, such as gallium phosphide (GaP), which are promising, but have not been widely explored. Innovative inverse design approaches may herald unprecedentedly flat and complex dispersion profiles, enabling synthesis of light of virtually any color on a chip, with any desired spectral envelope, in a fully coherent manner, at low powers—both pulsed and continuous wave.

There is an urgent need for optical materials that are widely tunable to enable light generation, manipulation, processing, and detection on a single platform. Current integrated optics platforms fall short. Silicon offers ideal compatibility with electronics, but it is a poor light emitter and a poor detector at telecom wavelengths, and it suffers from losses when it is modulated. III-V materials are excellent light emitters and detectors but lack compatibility with CMOS electronics for massive integration. Currently, heterogeneous integration of silicon photonics with bonded III-V materials represent the state of the art.

Two-dimensional materials can enable true monolithic integration of light generation, manipulation, and detection on a massively integrated platform with CMOS electronics (see Figure 2.6). These 2D materials are crystalline, comprise a single layer of atoms, and already have a breathtaking number of applications since their discovery in the early 2000s. In the past decade, room-temperature lasing, high-speed modulation, and high-speed detectors have been demonstrated using 2D materials integrated on photonic devices. The quantum confinement in the direction perpendicular to the 2D plane leads to novel electronic and optical properties that are not present in the bulk counterpart of these materials and other three-dimensional (3D) photonic materials such as gallium arsenide (GaAs) and silicon.

Graphene is a crystalline form of carbon in a sheet that is one atom thick. Graphene has unique optical properties such as a widely tunable refractive index and a zero bandgap, and it has been shown to be compatible with CMOS electronic manufacturing. Over the past decade, tremendous advances have been made in integrated detectors and modulators capable of more than 100 Gigabits per second bandwidths. Developing techniques to dope graphene are key to extracting its full potential. Graphene integration with deposited or amorphous materials enables a true electro-optic effect on otherwise passive platforms (e.g., silicon nitride,

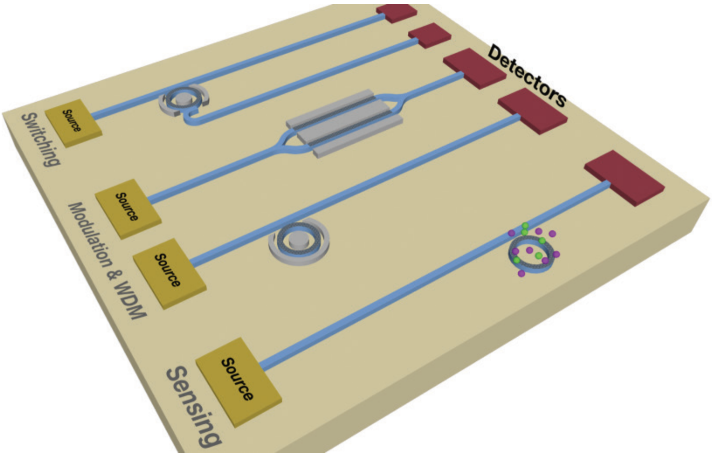

**FIGURE 2.6** Vision of two-dimensional (2D) photonic materials integrated with traditional dielectric and semiconductor materials. In a 2D photonics platform, passive structures can be integrated with novel active devices based on 2D materials. SOURCE: See the Cardenas Lab website at https://www.hajim.rochester.edu/optics/cardenas/gallery, used with permission from Prof. Jaime Cardenas.

silicon dioxide). It also enables low-power, large modulation in silicon without the carrier effects. Transition metal dichalcogenides (TMDCs), another 2D material, can be integrated with optical chips to enable generation of classical and quantum light. A recent demonstration of the presence of isolated defect single-photon emitters in 2D tungsten diselenide shows the potential of TMDCs to transform quantum information science. These single-photon emitters promise to be easier to integrate to photonic devices than their solid-state counterparts, such as NV centers in diamond. They are also expected to have higher tunability and sensitivity to ambient conditions. Yet another 2D material, black phosphorus, has a tunable bandgap that bridges those of graphene and TMDCs.

Integration of 2D materials with integrated optic platforms will transform the field of integrated optics and revolutionize communications, sensing, signal processing, and quantum information science, all important topics in AMO. It will enable integrated optics in three dimensions, where multiple photonic layers, each with its own sources, detectors, modulators, and sensors, can be monolithically integrated into a single electronic-photonic chip.

### Optomechanics

Optomechanics (OM) refers to systems in which there is transduction between light (as photons) and mechanical motion (generally as phonons). When laser light reflects off mirrors that are free to move, their mutual OM interaction is mediated by radiation pressure. Resonators, such as cavities, enable coupling of the light to and even cooling of the mechanical modes, as much as the atomic degrees of freedom. Stimulated by advances in nanofabrication and the quest for more precise measurements of force and displacement, OM interactions have been applied to probe fundamental quantum phenomena in objects over nano- to macro-size scales, and have opened up applications ranging from quantum information to precision quantum sensing.

OM interactions have been used to probe fundamental scientific questions such as, What is the ultimate limit to the precision of measurements? Where is the boundary between classical and quantum behavior? and How does decoherence manifest? On the more applied side, OM coupling on mass scales ranging from nanogram to gram have been deployed to create the tools of quantum information such as quantum memories for information storage and so-called hybrid systems for information transport. Other applications include quantum sensing of forces, displacements, spins, magnetic fields—for example, OM has also been used to create exotic quantum states of light—for example, squeezed light—and of mechanical motion—for example, phonon Fock states. Many phenomena that have been observed with light-atom interactions and with nonlinear optical systems have been replicated with light-mechanics interactions. OM research has both enabled and been enabled by technical advances in nanofabrication, cryogenic systems, and novel materials science and engineering.

The greatest impediment to realizing the full potential of OM interactions in the quantum regime is thermal noise of the mechanical oscillators. Most OM systems are cryogenically or laser cooled to mitigate the effect of thermal noise to reach the quantum regime. As nanofabrication technologies and the availability of low thermal dissipation materials improve, design and control of the mechanical oscillators will get more sophisticated. The lower thermal noise of future oscillators will allow quantum fluctuations to fully dominate the motion of the mechanical oscillators, perhaps even at room temperature. OM is a rapidly advancing field with a bright future.

### Attosecond Light Sources

In 2001, attosecond light bursts were first demonstrated in the laboratory using HHG in gases. This announcement meant that scientists now had a tool for following in time the electron motion in matter. Rapid progress in both attosecond source development and applications ensued. Table-top attosecond extreme ultraviolet sources (10 to 150 eV) driven by commercial Ti:Sapphire CPA lasers centered at 800 nm are now operating in many laboratories around the world. The typical repetition rate is 1 to 3 kHz. Over the past decade, the spectral range of high-order harmonics has been extended from the XUV into water window soft X rays

(282 to 533 eV) by exploiting the fundamental wavelength scaling toward higher HHG photon energy enabled by long-wavelength infrared laser drivers (>1.5 μm). Similarly, pulse durations have steadily decreased, with a current record of ~50 as. Figure 2.7 is a typical table-top setup for performing attosecond photoionization experiments. The principles of generating trains or isolated attosecond pulses are similar, and require only different shaping of the fundamental field. The concept of the apparatus is very similar to a synchrotron or XFEL platform: the attosecond source is the beamline, which can support different end-stations—that is, electron or photon detection—except in this case, it is all done in a laboratory-scale, ultra-high vacuum setup.

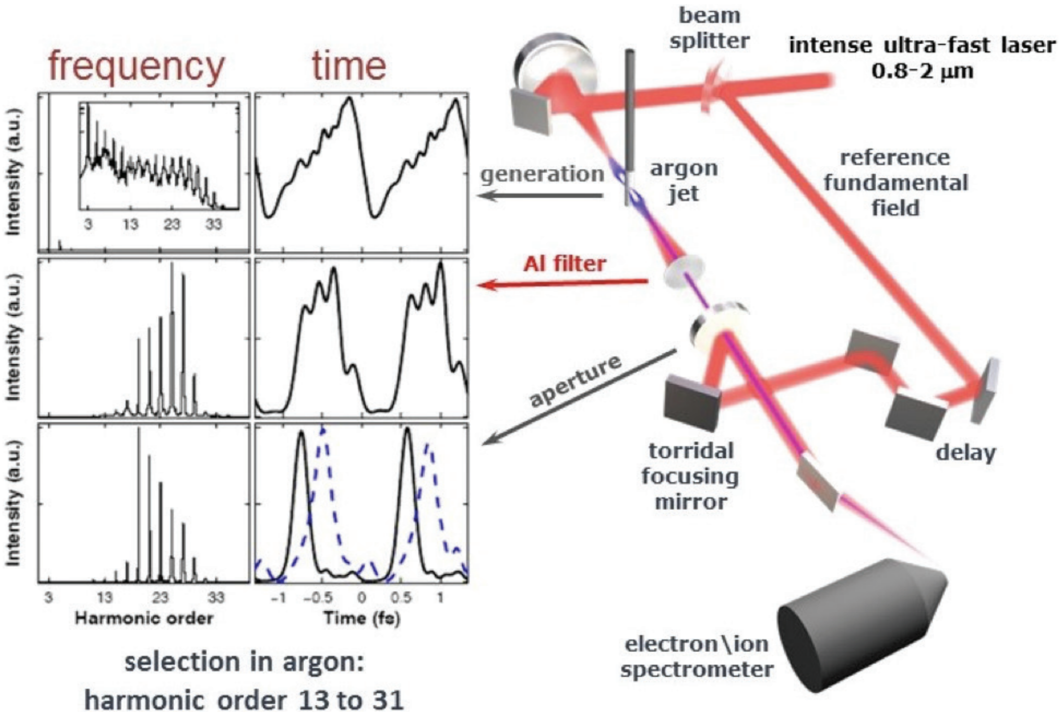

**FIGURE 2.7** A typical interferometric attosecond platform for RABBITT (Reconstruction of Attosecond Beating By Interference of Two-photon Transitions; described below). An ultrafast laser pulse is focused into a gas cell or jet producing phase-matched high-harmonic radiation. The harmonics phases are manipulated by spatial and frequency filtering. In this setup, the harmonics are focused into an electron spectrometer, where a suitable gas of interest is introduced. For transient absorption measurements, the end-station is replaced by a high-density gas or solid and an extreme ultraviolet monochromator/detector. A small portion of the laser energy is split off and sent down a second arm of a Mach-Zehnder interferometer. The spectrogram is recorded with attosecond precision by delaying the reference arm relative to the HHG arm. The panel to the left illustrates the progressive time-frequency relationships, and the formation of an attosecond train. An isolated pulse is formed on similar principles but requires a gating scheme on the reference laser pulse. SOURCE: Louis DiMauro.

In the next decade, attosecond X-ray open-access user facilities based on gas-phase HHG and XFELs will provide unique opportunities to scientists in many fields to study electron dynamics. The advances in high average power ultrafast laser sources offers a path for attosecond generation with significantly enhanced repetition rates spanning 0.1-1.0 MHz, allowing application of more sensitive detection schemes, such as multiparticle coincidence. Likewise, new high-power femtosecond mid-infrared lasers will enable the generation of kiloelectronvolt X rays with pulse duration approaching one atomic unit of time (24.2 as).

## HARNESSING THE PROPERTIES OF LIGHT

One of the strengths of AMO science is that the tools developed have broad impact on science and technology, which enables the development of new frontiers. One excellent example is the development of the optical tweezer by Arthur Ashkin (2018 Nobel Prize in Physics), a technique that has now become a standard tool in biology and atomic/quantum physics, but whose intellectual inception was understanding the basic principles of the light force. As elaborated throughout this study, this tradition continues to this day. This section illustrates how AMO scientists are harnessing the fundamental properties of light to generate new tools for metrology and sensing.

### Ultrafast X-ray Metrology

Since the beginning of the 21st century, our ability to measure light pulses has achieved a high degree of sophistication. Using the "zoo" of existing optical pulse characterization techniques, such as FROG, TADPOLE, and SPIDER,[6] researchers can precisely measure the spectral amplitude and phase of complex ultrafast light pulses. In addition, interferometric techniques based on nonlinear optics or photoelectron spectroscopy can determine the relative carrier envelope phase (CEP) of an ultrashort pulse with roughly 0.1 radian precision. In addition, the stereo-above threshold ionization phase meter method[7] can determine the CEP for a single shot, thus allowing the tagging of each individual laser pulse.

The challenge of moving ultrafast science toward shorter wavelengths is captured by a simple question: how do you measure the pulses' temporal properties? The AMO community has developed precise metrology for the complete

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[6] For a description of the optical methods see R. Trebino, K.W. DeLong, D.N. Fittinghoff, J.N. Sweetser, M.A. Krumbügel, and B.A. Richman, Measuring ultrashort laser pulses in the time-frequency domain using frequency-resolved optical gating, *Rev. Sci. Instrum.* 68:3277, 1997.

[7] The stereo-above threshold ionization method is a strong field photoionization technique for few-cycle pulses that is sensitive to small changes in the pulse's CEP.

characterization of optical laser pulses; these techniques are now being translated with the same level of sophistication into the XUV/X-ray regime. The cumulative research in strong field atomic physics has provided a means for retrieving the temporal information. In one variant known as RABBITT (Reconstruction of Attosecond Beating By Interference of Two-photon Transitions), the quantum interference of degenerate photoionization pathways results in modulation sidebands produced by XUV+IR fields. The resulting photoelectron spectrogram conveys information on the temporal structure of a train of attosecond pulses. Temporal measurement of isolated attosecond pulses uses a streaking method wherein the XUV attosecond pulse ionizes a target atom in the presence of a relatively intense, reference optical field. The freed photoelectron will receive an additional momentum kick from the reference field's vector potential, and this depends on the relative phase between the XUV and optical fields, controlled with an interferometer. Thus, the time-dependent vector potential of the reference field produces a trace similar to a conventional laboratory oscilloscope, except with a petahertz bandwidth. These techniques have gained wide acceptance for characterizing attosecond pulses from the XUV to soft X rays, and interrogating attosecond dynamics in nature. The clocking precision achieved in these measurements has achieved subattosecond performance.

The emergence in 2009 of the LCLS XFEL facility posed a new question for temporal metrology in the hard X-ray regime. How do you measure these short burst of X rays? The AMO community had the answer by translating the table-top techniques developed a decade earlier for measuring attosecond pulses. Although facility operation posed some interesting challenges for the application to the XFEL platforms, AMO scientists contributed to their solution, and in doing so had the opportunity for exploring new physics. These AMO techniques have become a staple on all XFEL facilities.

### Generation of Optical Clocks

Improvement of spectral resolution has been a key driver behind many scientific and technological breakthroughs over the past century, including the invention of the laser and the realization of ultracold matter. The development of optical atomic clocks in recent years has benefited from the same pursuit. A number of key ideas and enabling technologies have accelerated the progress of clock performance. These include the search for and use of exceedingly high-quality atomic transitions in the visible regime, quantum state engineering of single trapped ions and of many-atom systems in specially designed optical lattices, the development of ultrastable lasers, and the invention of optical frequency combs.

Precise control of optical phases is a dominant theme in laser science. In the spectral domain, continuous wave lasers are providing dramatically enhanced resolving power to see even finer energy structures of matter. Ultrastable lasers that maintain optical phase coherence for tens of seconds make it possible to investigate optical transitions with spectral resolution approaching 1 part in $10^{16}$. Through the powerful tool of optical frequency combs that unite stable optical phase control and ultrafast science, unprecedented spectral resolving power has been established across the entire visible spectrum and beyond.

Precise quantum state engineering of individual atoms has led to extraordinary measurement performance. The pioneering work of controlling single trapped ions for frequency standards has provided a rich set of scientific insights and technology advances. More recently, the use of many atoms, all confined in optical lattices with precisely engineered properties of trapping potentials that are independent of the two clock states, has greatly enhanced signal strengths for clock spectroscopy, leading to new levels of clock precision. The best atomic clocks have progressed to measurement uncertainty at the level of $10^{-18}$. Together with the progress of quantum matter and simulations, the prospect for further progress seems very promising. Furthermore, AMO scientists have created new opportunities for understanding and constructing quantum matter where many-body physics is no longer feared as a hurdle for precision measurement, but rather a new frontier to advance precision and accuracy. Shown in Figure 2.8 is the novel JILA 3D optical lattice clock, which contains a quantum gas of fermionic atoms that are spatially correlated to guard against motional and collisional effects. This type of system will provide a powerful platform to integrate many-body quantum state engineering with quantum metrology, creating exciting opportunities to advance precision beyond the standard quantum limit.

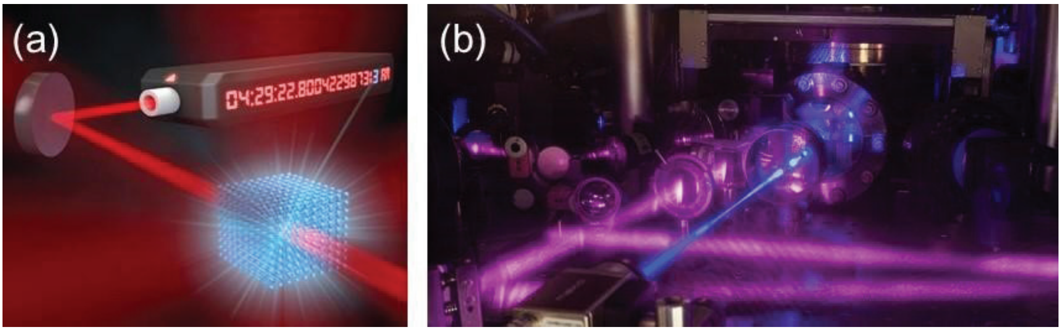

**FIGURE 2.8** (a) A three-dimensional optical lattice quantum gas atomic clock consists of a grid of light formed by three pairs of laser beams. (b) A blue laser beam excites such a cube-shaped cloud of strontium atoms located behind the round window in the middle of the table. Strontium atoms fluoresce strongly when excited with blue light. SOURCE: (a) Courtesy of JILA and Steven Burrows; (b) NIST, "JILA's 3-D Quantum Gas Atomic Clock Offers New Dimensions in Measurement," News, October 5, 2017, https://www.nist.gov/news-events/news/2017/10/jilas-3-d-quantum-gas-atomic-clock-offers-new-dimensions-measurement; courtesy of G.E. Marti/JILA.

The convolution of precision control of light and matter is helping bridge different disciplines in physics and fostering new capabilities to probe fundamental and emerging phenomena. Many new scientific frontiers (see Chapter 6) have emerged and are being elucidated through the quest of building a better atomic clock, for example, tests of fundamental physics, the development of sensors of increasing sensitivity, the probe of quantum many-body physics, and the search for new physics beyond the standard model.

### Light Propagation: Sensing and Control

The highly directional character of laser beams makes them ideal for remote (long distance) detection of chemical pollutants on the one hand, and for distance surveying on the other hand—for example, for mapping or use by autonomous vehicles. There are many examples of AMO-derived sensing technologies that have given rise to profound impact on environmental and other monitoring activities. An important application is the use of optical fibers to measure physical, chemical, and bio/medical phenomena. Fundamental progress in the understanding of light propagation, relativistic interferometry, the band structure of ions in glassy media, and absorption/scattering processes in "exotic" optical media have all contributed to the success of fiber optic sensors in civilian and defense applications.

A traditional approach to remote detection involves Laser-Induced Breakdown Spectroscopy (LIBS). In LIBS, a laser beam creates a small plasma plume on some remote target. As the plasma recombines, the constituents emit characteristic frequencies that can identify the materials spectroscopically. Two problems exist: (1) during propagation, laser light spreads, producing a lower intensity on target; and (2) the emitted recombination light suffers a large radial loss as it propagates back to the remote detector.

Recently, an exciting alternative to LIBS was developed. An ultrashort laser pulse propagating through the atmosphere will have sufficient peak power to drive the nonlinear effect of filamentation. In light filamentation (LF), the air acts like a lens, and focuses the laser down to the point where air molecules are ionized and a plasma forms; the plasma arrests any further spatial collapse, and the competing interactions result in stable propagation of a coherent light/plasma beam. LFs have extraordinary properties: (1) they do not diffract, thus producing high-intensity beams on distant targets; and (2) their coherence spans the entire visible range making them ideal for spectroscopic analysis.

Recent research has shown LFs can create terahertz (THz = $10^{12}$ cycles/s) radiation at the remote target. Terahertz radiation is important for spectroscopic analysis but does not propagate well through the atmosphere. LFs create the terahertz energy near the target, thus minimizing atmospheric loss. In addition, LFs can produce a local disruptive electromagnetic pulse. Recently, the Army Research Office demonstrated remotely disabling a drone from one shot of an LF.

In the future, new schemes of light/plasma interactions on distant targets are expected. Researchers are exploring air lasing to create backward-propagating beams, which would alleviate the propagation loss. Additionally, a unique solution to Maxwell's equations supports a "flying torus" structure, which is quite unlike a conventional electromagnetic wave. In such structures, the magnetic field consists of loops, the plane of which are perpendicular to the direction of propagation, and the electric field wraps around the magnetic field. Although theoretically known for some time, flying torii have eluded generation and detection.

Another recently emerged powerful technique for broadband spectroscopy and sensing is laser frequency combs. While initially developed for frequency metrology, frequency combs have become a powerful tool for new approaches to broadband molecular spectroscopy. The broad coherent spectrum of sharp comb lines permits novel approaches to linear and nonlinear spectroscopy that often outperforms other state-of-the-art techniques with respect to resolution, accuracy, recording time, and sensitivity.

Comb laser beams enable both local sensing at very high sensitivity and integration over columns of kilometers of open path. The broad spectral bandwidth enables simultaneous interrogation of multiple species and transitions, improving the consistency and reliability of measurements. When comb lines are resolved, the contribution of the instrument to the experimental line profiles becomes negligible. A number of proof-of-concept demonstrations of broadband frequency comb spectroscopy for sensing applications already highlight its great potential. A dual-comb spectrometer operated in the mid-infrared spectral region can achieve open-path monitoring of ammonia from tens of meters away on millisecond time scales. Similarly, open-path comb-based mid-infrared measurements achieved detection of atmospheric $CH_4$ and $H_2O$ on millisecond time scales. Comb spectroscopy has also been employed to measure the concentration of radicals involved in the atmospheric chemistry of the marine boundary layer such as BrO, IO, and $NO_2$ on minute time scales and with detection limits better than 10 parts per trillion volume in East Antarctica.

More recently, dual-comb spectroscopy with resolved comb lines interrogated atmospheric trace gases with high sensitivity over a 2-km open-air path, retrieving path-integrated concentrations of several greenhouse gases with remarkable consistency across repeated measurements. With continued progress in fiber laser technology, comb-based spectrometers are now transportable. Field-deployed instruments have been successfully used to make measurements in an industrial gas turbine, and identify and quantify leaks from methane sources over multiple-square-kilometer regions at emission rates three orders of magnitude lower than conventional approaches. Furthermore, other sampling techniques may diversify the tools for spectroscopic diagnostics. For instance, the combination of laser-induced breakdown spectroscopy and dual-comb spectroscopy lays the groundwork for in situ analysis of soils, rocks, and minerals.

## THE FUTURE FOR NEW TOOLS MADE OF LIGHT

History has shown the transformational impact on science, technology, and society enabled by advances in light engineering. Whether it was the discovery of X rays by Röntgen, the first demonstration of the laser by Maiman, or the development of an efficient blue diode by Akasaki, Amano, and Nakamura, the global impact on society is immeasurable. Based on the emergence of novel light capabilities inspired by grand challenge needs in science, it is easy to predict a continuation of transformational impact.

Given the amazing capabilities in the control of optical coherence, manifested in either the spectral or temporal domains, light-matter interactions are entering a new phase to drive new scientific discoveries and novel technology development. The light's high temporal and spatial coherence makes it possible to produce waveforms that span the infrared, visible, ultraviolet, and even soft X-ray spectral regions. In the spectral domain, continuous wave lasers are providing dramatically enhanced resolving power to see ever finer energy structures of matter. Ultrastable lasers that maintain optical phase coherence for many seconds make it possible to investigate optical transitions with resolution better than 1 part in $10^{15}$. Many new scientific thrusts have emerged from that quest, such as testing for fundamental symmetries, developing sensors of increasing sensitivity, probing the quantum nature of many-body physics, and searching for new physics beyond the standard model. The best atomic clocks are now based on stable light interacting with precisely controlled atoms and ions. These systems have strong potential for continued progress in the coming decade.

The production and control of quantum states of light will play critical roles in the emerging networks of quantum communication, as discussed in Chapter 4. At the same time, the squeezed state of light is already employed to reduce quantum noise in the current gravitational wave detectors at the Laser Interferometer Gravitational-Wave Observatory (LIGO), significantly improving the detection sensitivity of compact binary coalescences. The development of platforms that combine quantum information science and integrated photonics will greatly advance the applications, sensing, communications, and computing.

Watching, clocking, and controlling all the constituents of matter remains a dream of science, having been an active area of research for several decades. The progress has been steady and insightful, but the dream remained just that. However, several recent developments in ultrafast X-ray science could provide a turning point in realizing the dream (see Chapter 5). First, the continued advances in attosecond science and technology are providing visualization of the fastest constituent of matter, the electron. The emergence of high-average-power ultrafast lasers will now enable high-fidelity measurement tools for watching this movement. Second, the development of XFEL facilities are a revolutionary concept that brings "ultrafast" into the vernacular of X-ray science. The well-known utility of X rays for determining molecular structures will now record molecular movies. It is expected that as both technologies progress, the next decade could see the realization of the dream.

The frontier of intense laser-matter interactions has seen a major increase in activity. The holy grail is to reach sufficiently high intensity to break the vacuum: to create something from nothing. The current state-of-the-art laser is seven orders of magnitude too low to achieve that now except with the Lorentz transformation using ultra-relativistic electron accelerators. However, efforts in Europe and Asia are pushing the technology to raise the highest power obtainable from a laser into the tens of petawatt range and beyond. These laser developments need a facility-type environment for operation and thus significant investment. The U.S. funding for this frontier has lagged behind, but recent federal activity in response to the 2018 National Academies of Sciences, Engineering, and Medicine report *Opportunities in Intense Ultrafast Lasers*[8] could improve the landscape in the United States. This investment will be central for the United States to regain some leadership in an area that has important national security consequences. The XFELs have an additional transformative and unique quality at X-ray frequencies—extraordinary intensity. This raises another frontier question: how does an intense X-ray pulse interact with matter? The only thing that is known is that it will be dramatically different from known interactions using visible lasers. In fact, this regime may not be compatible with current theoretical approaches, and will largely be pioneered by experiments. As the XFEL engineering improves performance, and as new facilities in Europe and Asia increase accessibility, it may be possible to begin the exploration of this physics, some of which is highlighted in Chapter 5.

## FINDINGS AND RECOMMENDATIONS

**Finding:** The past decade has seen revolutionary advancements in ultrafast light source development spanning the XUV and X-ray spectral regime. The ability to control and manipulate these tools made of light is enabling new applications that extend beyond AMO physics. New platforms are emerging in quantum information science, remote sensing, and clocking ultrafast electron dynamics in all phases of matter. Thus, the frontiers lie at the interdisciplinary intersection of physics, engineering, chemistry, materials science, and biology.

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[8] National Academies of Sciences, Engineering, and Medicine, 2018, *Opportunities in Intense Ultrafast Lasers: Reaching for the Brightest Light*, The National Academies Press, Washington, DC.

**Finding:** Advances in ultrafast X-ray science has become increasingly demanding of resources that are beyond the ability of single principal investigator (PI) funding models. XFELs are large-scale facilities that need the management infrastructure of a National Laboratory. However, table-top systems, such as attosecond- and petawatt-class lasers, have evolved to the level of a mid-scale facility requiring operational management and safety infrastructure. The United States has lagged behind the rest of the world in capitalizing on the opportunities enabled by these mid-scale facilities, training of a workforce at the cutting edge of technology, and the economic benefits of industrial growth.

**Key Recommendation: U.S. federal agencies should invest in a broad range of science that takes advantage of ultrafast X-ray light source facilities, while maintaining a strong single principal investigator funding model. This includes the establishment of user facilities in mid-scale university-hosted settings.**

**Finding:** Despite the enormous advances of integrated linear and nonlinear photonics based on silicon, there is a need for ultra-low-loss platforms where light can be generated with ultrahigh efficiency, switched and detected, especially for quantum-related applications. Such a platform would probably be formed via the integration of multiple materials on silicon.

**Finding:** Systems exhibiting strong photon-photon interactions are currently being explored, to enable unique applications such as quantum-by-quantum control of light fields, single-photon switches and transistors, all-optical deterministic quantum logic, the realization of quantum networks for long-distance quantum communication, and the exploration of novel strongly correlated states of light and matter.

**Finding:** As nanofabrication technologies and the availability of high optical quality, low thermal dissipation materials improve, design and control of the mechanical oscillators will get more sophisticated. The lower thermal noise of future oscillators will allow quantum fluctuations to fully dominate the motion of the mechanical oscillators, perhaps even at room temperature, creating a versatile quantum resource for a variety of applications.

**Key Recommendation: The federal government should provide funding opportunities for both basic and applied research that enable the development of industrial platforms, such as foundry offerings, and interdisciplinary academic laboratories to support the integration of photonics and engineered quantum matter.**

# 3

# Emerging Phenomena from Few- to Many-Body Systems

## INTRODUCTION

In any typical gas at room temperature, the molecules are zooming around randomly and colliding more or less like billiard balls according to the laws of Newtonian mechanics. In this physical regime, the motion of the molecules is exemplified by chaos, which continues to be a subject of inquiry for atomic, molecular, and optical (AMO) researchers. But in order to display quantum mechanical behavior, the experimenter must cool the gas down to ultralow temperatures, below 1 microkelvin—that is, below one millionth of a degree above absolute zero. The use of lasers, magnetic fields, and other tools to reduce the temperature of a gas from room temperature down to this submicrokelvin range has become routine for many atomic species and even for some molecules. The figure of merit is the ratio between the average interparticle distance ($d$) and the quantum de Broglie wavelength ($\lambda$); when $d/\lambda$ falls to the order of unity or less, a collection of particles is deep in the quantum regime in which the dual particle and wave natures of the system become important. In this fascinating regime, quantum phenomena that challenge our intuition become commonplace.

This chapter focuses on describing the advances in experimental control that have produced realizations of a broad range of quantum mechanical phenomena, for as few as two atoms, up to many-particle systems with thousands or even millions of atoms or molecules. These research activities have enabled a deeply satisfying intellectual pursuit to understand quantum complexity from the ground up, while at the same time providing a fertile playing field in which to connect precisely controlled atomic and molecular systems. While this sometimes involves understanding the addition of one atom at a time, this research track ultimately connects with the interests of a number of subdisciplines in physics, including condensed-matter physics, precision measurement, chemical physics, and quantum information. Just as Chapter 2 describes the essential research tools based on the control of photons, this chapter provides an overview of how individual atoms, once brought under precise control, become both a fascinating subject for study and an enabling technology for a range of frontier research topics. Figure 3.1 gives an overview of the topics revolving around ultracold science that are discussed in this chapter.

All of the topics discussed in this report are challenging and have a frontier at the very edge of what is known and understood. Many of the phenomena being discussed are *complex*, but this is a word with multiple meanings. Some systems are complex because they consist of many particles, and because new phases emerge that have no counterpart whatsoever for small numbers of particles. On the other hand, even some systems of two particles can be tremendously complex, for instance if they involve atoms in the lower half of the periodic table, with electronic configurations that are not all closed shells, and with a huge number of internal

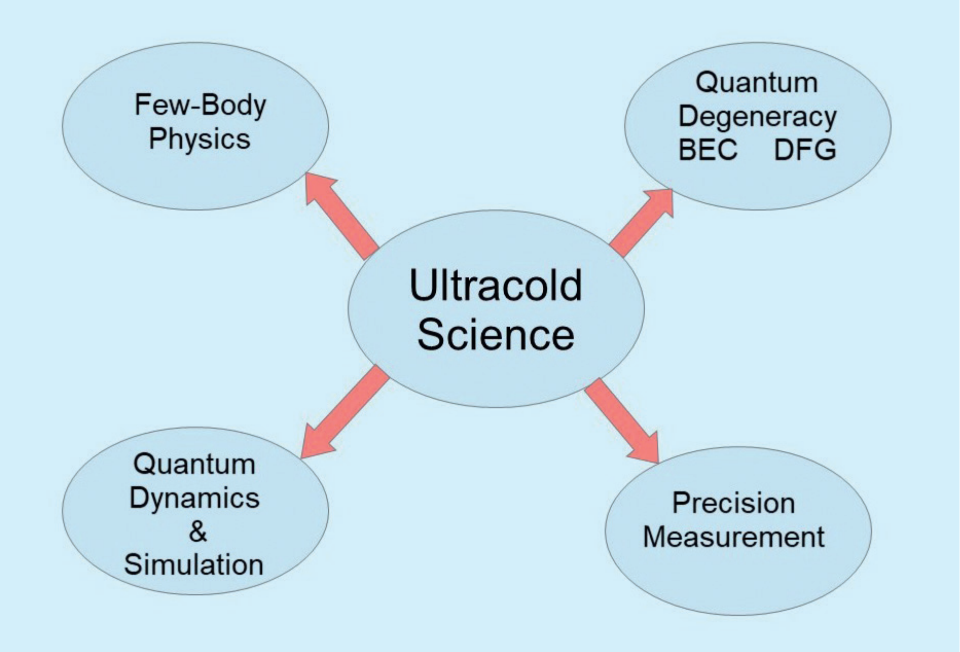

**FIGURE 3.1** Topics centered on ultracold science that are discussed in this chapter. NOTE: BEC, Bose-Einstein condensate; DFG, degenerate Fermi gases. SOURCE: Chris Greene.

states that have nearly the same energy. And yet another meaning of *complexity* is what the chaos community identifies with and studies in all of its ramifications relating to randomness of trajectories or motions: in the classical Newtonian world chaotic complexity takes one form, but it has different manifestations in the quantum world.

Atoms come in two "flavors," boson and fermion. Fermions cannot be in the same state at the same time—they must avoid each other. Bosons on the other hand have a well-known tendency to group together in the same quantum state. In the 1990s, bosonic atoms like rubidium were cooled down to the quantum regime to form a new phase of matter, the Bose-Einstein condensate (BEC), in which nearly all the atoms congregate into a single wave-like state. Soon afterward, fermionic atoms like the 6-nucleon isotope of lithium ($^6$Li) were cooled down to a different quantum regime called the degenerate Fermi gas (DFG). In this regime, further cooling the fermionic atoms does not cause them to slow down—they have to keep moving so that they are all in different states. Following that period when these types of quantum degenerate gases were first created and initially explored, a fertile period of more than a decade followed, in which other types of mixtures were formed, and tunability using magnetic or electromagnetic fields proved that interactions between the constituent particles can be exquisitely controlled in the laboratory. This resulting remarkable level of interaction control enabled a further revolution in ultracold science, including the creation of dynamical phenomena such as solitons and vortices. Moreover, the advent of laser-formed optical lattices, in which light waves form a periodic array in space that traps atoms in those periodic arrays, resembles the physics of a crystalline environment seen by electrons in solids. During the past decade, this collection of experimental techniques has enabled access to an increasingly rich array of phenomena and the creation of novel phases of matter. In many cases, these phenomena are fascinating to study in their own right, while in other cases their value derives from the ability to simulate novel phenomena in condensed-matter and topological physics with an unprecedented level of control.

Recent years in the field of ultracold quantum gases have seen remarkable achievements. BECs and other types of quantum degenerate systems have reached such a high level of control that they can now be created in the laboratory across a rich variety of situations (in one-, two-, or three-dimensions, for instance, and in uniform quantum fluids or in the crystalline environment of an optical lattice), and for many different chemical elements; they can even be created on a satellite in outer space. The controllability of the deep quantum world continues to grow in leaps and bounds, spreading throughout the atomic periodic table of elements, and increasingly into the far richer and more diverse arena of ultracold molecules. The latter pose tremendous practical challenges, since the complex electronic, rotational, and vibrational modes of molecules are not nearly as well understood nor as easy to control as the relatively simple modes of single atoms. This additional complexity makes molecules often less well suited to laser cooling and trapping (though rapid improvements in these techniques are ongoing).

Many of the experimental tools developed to understand and control atoms and molecules in ultracold environments have progressed to the level where they can now be used to simulate interesting and nontrivial quantum systems, such as the Fermi-Hubbard model that describes the behavior of quantum magnets and high-temperature superconductors. As discussed below in the section "Analog Quantum Simulation of Strongly Correlated Quantum Many-Body Systems," this type of quantum simulation has the potential to simulate the behavior of systems that are currently beyond our ability to treat reliably using existing theoretical methods or computers. Such applications are at the forefront of current quantum information applications. Quantum simulation represents a promising science direction in its own right, while others appreciate developments in that subject as stepping-stones along the route to quantum computing applications, discussed at greater length in Chapter 4.

## FROM FEW BODIES TO MANY BODIES: HOW COMPLEXITY BUILDS

Science has an innate tendency toward the discovery and understanding of more and more detailed phenomena, in virtually all areas. Examples of this abound, such as the fabrication and cataloguing of ever more specialized materials and metamaterials designed to affect light in increasingly specialized ways, or to unraveling the behavior of different types of quantum gases, consisting of different atoms, different molecules, different spin statistics (bosonic and fermionic), different topologies, or different spatial dimensions. At the same time, AMO physics shares a goal with many other disciplines—namely, to extract universal truths that persist across different systems, with a common physical origin, but differing in some cases by orders of magnitude in their length, mass, and energy scales.

The simplest example of such universality arises already with the interaction of a pair of particles, deep in the low-energy quantum mechanical regime where the quantum wavelength is the longest length scale in the problem. Pioneers of quantum physics such as Fermi, Bethe, and Schwinger showed that a single quantity, the scattering length, controls the way two particles interact at low energy, and in some cases, form a weakly bound state. The early successful theoretical descriptions of degenerate quantum gas experiments—for example, in the mid-1990s and afterward—made use of this fact because the behavior of quantum gases depended almost entirely on the scattering length, and simple scaling with mass or trapping potential strength. The tremendous chemical differences, say, between atomic helium and rubidium, turned out to be irrelevant for the description of their BECs, as it was only the atom-atom scattering length of the system that mattered. In the late 1990s, AMO physicists demonstrated the ability to manipulate those scattering lengths at will, through the technique of magnetic Feshbach resonances. This technique ushered in a whole new era of controllable quantum gases that has continued robustly to this day.

This exquisite control of atom-atom interactions has launched studies in a strikingly rich and diverse array of systems. Experiments and theory relating to novel few-atom quantum states have seen tremendous progress during the past decade. For instance, the magnetic controllability of interactions enabled the first observation in 2006 of the intriguing, counterintuitive quantum states known as "universal 3-atom Efimov states," and many subsequent experiments have similarly used magnetically tuned resonances to observe Efimov trimers in both homonuclear and heteronuclear cases. The word "universal," used in this context, refers to the fact that any three-particle system with limited range but strong interactions (i.e., large scattering lengths) should have such states. Moreover, in the past few years, the first naturally occurring case of an Efimov resonance was observed experimentally for three very weakly bound helium atoms; that impressive experiment combined cold atom source and detection technology with ultrafast lasers to detect the size, shape, and binding energy of the delicate bound state. Box 3.1 gives some more details about this remarkable helium trimer system and its experimental observation. Additional, somewhat related families of universal quantum states consisting of four ground-state atoms have also been predicted theoretically and observed in experiments, with extensive progress and current interest in extensions of such studies to find universal states involving more than four atoms.

Microscopically, atoms interact predominantly in a pairwise manner, but multibody interactions can emerge in contexts such as three-body recombination processes, including for example Efimov states and other forms of universality associated with long-range interactions. Multibody interactions have also been observed in bosonic systems in optical lattice experiments. For fermions, a single impurity interacting with a few identical fermions has been studied (see Figure 3.2.1 in Box 3.2), and recently multibody interactions in high-spin fermions have been explored in individual lattice sites of an optical lattice.

Another developing area has been looking at few-atom or few-molecule physics in optical tweezers. Optical tweezers are focused laser beams that attract atoms to the region of highest light intensity, thereby trapping them in a potential well. One interest is to create double-well potentials using a laser electromagnetic field, and then to observe entangled tunneling events, which yield insight into the effect of quantum entanglement on dynamical processes. (The concept of entanglement is discussed more fully in Chapter 4.) A second type of experiment observes an individual chemical reaction event of two molecules in a single potential well. In yet another kind of experiment, optical tweezers have been used to study entanglement physics involving highly excited Rydberg states of trapped atoms, as is discussed later in Chapter 4.

## BOX 3.1
## Naturally Occurring Three-Atom Universal Efimov Effect Observed Experimentally

Any two ground-state atoms in the periodic table attract each other to some degree, but only if the attraction has some minimal strength can two such atoms bind together into a stable diatomic molecule. In the intriguing, highly nonintuitive Efimov effect (named after Russian nuclear theorist Vitaly Efimov, who predicted this effect in 1970), some remarkable properties emerge when one brings a third weakly attracting atom into the system. For instance, a situation exists for some weakly attracting atoms where the force of attraction is too weak to bind two atoms together, but when the third atom is introduced, there is enough extra force to hold all three together as a stable triatomic molecule. Such a system that has a bound trimer but only unbound dimers is sometimes referred to as "Borromean" because of the analogy to the so-called Borromean rings depicted in Figure 3.1.1 (panel A), where the three rings are held together but no two rings would remain connected by themselves. Another surprising feature of this odd corner of the quantum mechanical world of three weakly attracting particles is that there is one condition (infinite two-body scattering length) for which there are predicted to be an infinite number of these so-called Efimov states even though no stable dimer states exist. The first experimental observation of an Efimov state was made in 2006 by a group in Innsbruck, Austria, created by artificially manipulating the scattering length between ultracold cesium atoms. Several years later, experimentalists in Frankfurt demonstrated that atomic helium possesses such an Efimov state naturally, without requiring this artificial modification of the inherent force field. Figure 3.1.1 (panel B), shows the experimental evidence for two bound trimer states in this weakly bound system of three helium atoms, where the lowest energy (non-Efimov) trimer state of $He_3$ is observed to have far smaller atom-atom bond lengths than in the observed excited state $He_3^*$, which fits theoretical predictions for an Efimov state.

Ultracold physics has enabled the experimental observation of other peculiar types of few-body quantum states bound together into stable (or metastable) molecules via novel mechanisms. For example, once an electron in an atom is excited to a very high lying (Rydberg) state, it orbits slowly at a large distance from the nucleus, much as Pluto takes many Earth-years to orbit the Sun. It turns out that an atom in a Rydberg state can attract a nearby ground-state atom and create an ultra-long-range "Rydberg molecule." Some of these quantum states are predicted to exhibit a striking electron probability distribution that resembles a trilobite fossil, while others show a resemblance to a butterfly. Over the past few years, experimental observations of Rydberg molecules with huge internuclear distances have multiplied, even including observation of the trilobite and butterfly molecules whose creation poses stringent challenges. Another type of diatomic molecule with still larger internuclear distances has been predicted and observed, a so-called macro-dimer, made of two Rydberg atoms bound to each other through very-long-range interactions. These interactions result from each of the slowly orbiting outer electrons strongly perturbing each other through the Coulomb force.

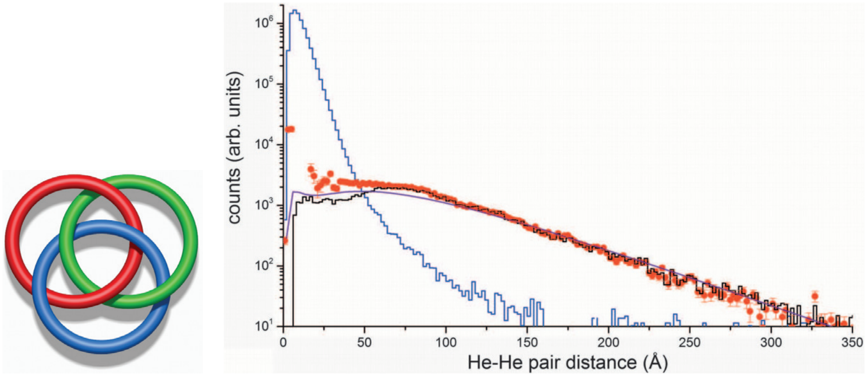

**FIGURE 3.1.1** Distribution of experimentally measured distances (deduced from detected coincidence ion counts) between two helium atoms in the ground state (blue) and first excited state (red and black, the Efimov state, measured two different ways) of three helium atoms, compared with current theoretical predictions (purple) for the excited state. Note that the average distance between any two atoms in this three-atom Efimov state is around two orders of magnitude larger than the size of a single bound pair, confirming the bizarre quantum mechanical nature of this universal binding mechanism. SOURCE: *Left:* Jim.Belk, "3D Borromean Rings.png," March 23, 2010, https://commons.wikimedia.org/wiki/File:3D_Borromean_Rings.png. *Right:* From M. Kunitski, S. Zeller, J. Voigtsberger, A. Kalinin, L.Ph.H. Schmidt, M. Schöffler, A. Czasch, W. Schöllkopf, R.E. Grisenti, T. Jahnke, D. Blume, R. Dörner, Observation of the Efimov state of the helium trimer, *Science* 348(6234):551-555, reprinted with permission from AAAS.

More detailed spectroscopy of such diatomic and analogous triatomic molecules has already revealed striking physics, such as huge electric dipole moments (thousands of times larger than in typical molecular ground states), which enable controllability by very small external fields. This area remains ripe for future explorations. Another direction for such studies comes from adding two, three, four, or even more ground-state atoms bound to a single excited Rydberg atom. For this class of systems, theory and experiment have begun to indicate the manner in which the bulk limit emerges, where very many ground-state atoms interact with, and in some cases even bind to, a single Rydberg atom.

## ULTRACOLD PHYSICAL PROCESSES INVOLVING IONS

Charged particles experience far stronger forces in an electromagnetic field than the neutral atoms and molecules discussed in the preceding portion of this chapter. But in the blink of an eye, a neutral atom or molecule can be turned into a positively charged ion, simply by striking it with a laser beam of an appropriately

## BOX 3.2
## Formation of a Fermi Gas, One Atom at a Time

In yet another application that connects few-body and many-body physics, it has been demonstrated that one can create a degenerate Fermi gas of atoms by adding atoms to a single one-dimensional potential well, one atom at a time, as Figure 3.2.1 illustrates. The use of optical tweezers to investigate fundamental few-particle entanglement and dynamics has been a growth area in recent years, and it is ripe with opportunities for the coming decade.

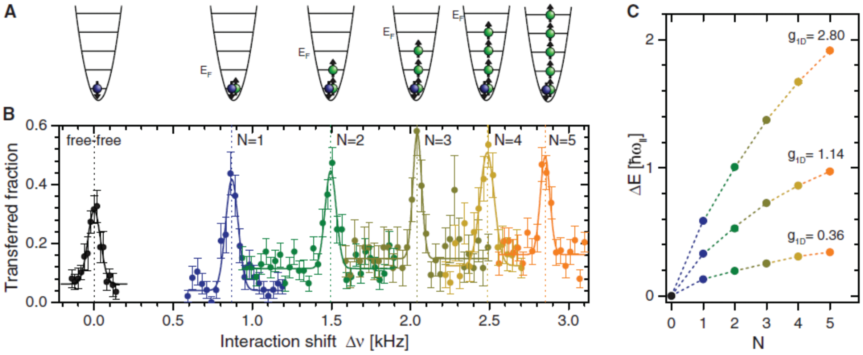

**FIGURE 3.2.1** Formation of a Fermi gas, one atom at a time. (A) Deterministically prepared noninteracting (N + 1)-particle states in a one-dimensional system of fermionic lithium atoms. (B) Measured radiofrequency spectra for a single impurity (a spin down lithium atom) interacting with different numbers of majority atoms with spin up. SOURCE: From A.N. Wenz, G. Zürn, S. Murmann, I. Brouzos, T. Lompe, S. Jochim, From few to many: Observing the formation of a Fermi sea one atom at a time, *Science* 342:457, 2013, reprinted with permission from AAAS.

chosen frequency and intensity that ejects one or more of the atom's electrons. A subject of fundamental interest that also has significant practical importance is how a system of positive ions and electrons behaves, and how it can be controlled and directed to behave under a wide variety of conditions. Such explorations are often viewed as the purview of the field of plasma physics, but they overlap significantly with atomic and molecular physics as well. During the past two decades, new insights into the behavior of plasmas have been derived by creating plasmas at ultracold temperatures by first cooling atoms to microkelvin temperatures and then using a laser to ionize a large fraction of the atom sample. Ultracold plasma physics has made several key strides during the past decade. Box 3.3 gives an indication for the progress in this area of research.

Ions of an atom or a molecule have numerous additional dynamical roles beyond those that arise in ultracold plasmas. One example that has been studied extensively by theory and experiment during the past decade is the system of one or a few ions placed in an ultracold quantum gas of neutral atoms. This is an ultracold variant of a process that occurs continually in nature—for instance, when a cosmic ray particle ionizes an atom in living tissue or in a computer chip, and subsequently affects the nearby neutral molecules. On the face of it, immersing a single trapped ion in the midst of 100,000 or so atoms, say of a BEC, might seem to have only a minor effect on the atom cloud. In fact, however, a rather violent series of events occurs, because the atoms are attracted to an ion orders of magnitude more strongly than to each other. As a result, the atoms nearest to the ion are drawn in and collide with the ion. When two free atoms (e.g., Rb) collide simultaneously with the ion (e.g., $Ba^+$), the ensuing three-body recombination process $Rb + Rb + Ba^+ \Rightarrow BaRb^+ + Rb$ converts the atomic ion to a molecular ion, and in the process adds sufficient kinetic energy to the free Rb atom to eject it from the condensate. If the molecular ion remains trapped, as is usually the case, the three-body process can repeat and create a heavier molecular ion, $BaRb_2^+$ while ejecting a second Rb atom from the condensate. This sequence of reactions can occur rather rapidly, and fundamentally change the initially quiescent Rb BEC into a roiling, highly excited, collection of residual atoms that are no longer even quantum degenerate. Studies in recent years have unraveled many of the details of this process, and shown various ways to control it—that is, how to either encourage such reactions or suppress them.

Another fascinating dynamical regime that has been achieved through separation of charge in a BEC occurs when a single atom in the middle of a large BEC is laser excited to a very high Rydberg state, whose size can be comparable to that of the entire BEC. The roaming Rydberg electron, as it moves through the three-dimensional (3D) atom cloud, can now interact with all the atoms in the BEC, producing energy shifts, while at the same time triggering the process of associative ionization—for example, $Rb + Rb^* \Rightarrow Rb_2^+ + e$. This can also have a significant effect on the behavior of the rubidium atomic condensate, owing to the energy deposited into the cloud.

Cooling and trapping of ultracold molecular ions is another topic that has advanced rapidly in recent years, and this is being pursued with a number of different long-term goals. Some of them are focused on precision physics tests of fundamental symmetries of the universe, including measurements of the electron electric dipole moment or of the electron to proton mass ratio to explore the possibility of a time-dependent ratio. (More on such precision tests can be found in Chapter 6.) Other applications of ultracold molecular ions arise and are of interest in basic spectroscopic and chemical reaction studies with fully defined preparation and observation at the individual quantum level, and the study of ion-neutral collisions is important for sympathetically cooling the ions. Cold molecular ion reactions are also important for understanding classes of astrophysical processes.

### BOX 3.3
### Ultracold Neutral Plasmas

Ordinary neutral plasmas typically exist at temperatures in excess of 1,000 K, which is set by the energy required to sustain collisional ionization. However, by photoionizing laser-cooled atoms with a pulsed laser whose frequency is tuned near the ionization threshold, it is possible to create ultracold neutral plasmas, with temperatures as low as about 1 K. Theory and experiment have investigated many different aspects of these novel systems, such as equilibration after plasma creation and collisional formation and ionization of Rydberg atoms. Because the strength of the Coulomb interaction is large compared to the thermal energy, ultracold neutral plasmas have also become a powerful platform for studying dynamics and transport in strongly interacting plasmas.

In a strongly interacting plasma, the Coulomb interaction energy between neighboring particles exceeds the average kinetic energy. This leads to the development of short-range spatial correlations that modify collective modes and collision rates. Ongoing research is focused on developing a complete theoretical description for plasmas in this regime. Experiments with ultracold plasmas provide valuable benchmarks for development of new theoretical techniques and for validation of molecular dynamics simulations. These efforts may improve our understanding of other systems that can be described as strongly coupled plasmas, such as white dwarf stars and inertial-confinement-fusion plasmas.

In a recent advance, laser cooling was applied to ions in an ultracold neutral plasma (Figure 3.3.1), reversing the order of cooling and ionization, yielding ion temperatures as low as 50 mK and making the system even more strongly coupled. Laser forces are strong enough to retard or enhance the plasma expansion into the surrounding vacuum, suggesting new possibilities for neutral-plasma confinement. Magnetized ultracold neutral plasmas is yet another active area of investigation because of the connection to plasma confinement (e.g., for fusion energy) and for what can be learned about modification of recombination dynamics in strong fields. Photoionization of laser-cooled clouds of multiple atomic species yields more complex, strongly coupled plasmas, which are being studied to investigate phase separation and interspecies thermalization. Ultracold neutral plasmas are also formed by photoionizing molecules that

## DEVELOPMENTS WITH ATOMIC DEGENERATE QUANTUM GASES

Once atoms have been cooled down to temperatures in the range 1-100 nanoK, new states or phases of matter have been predicted to occur, and by now many novel phases have indeed been created and observed. Some of these are quantum versions of classical nonlinear wave phenomena, such as solitons (solitary waves) and vortices, and even neatly aligned arrays of vortices. The atoms carry spin degrees of freedom, which perform their own dance, either separately or in some cases in controlled concert with the motional degrees of freedom.

Interacting unexcited (ground state) atoms are the usual constituents of degenerate quantum gases—namely, BECs, DFGs, and mixed systems. Recent developments in the field of dilute quantum gases have included some of the first explorations of a BEC in the limit where the atom-atom interaction has been tuned

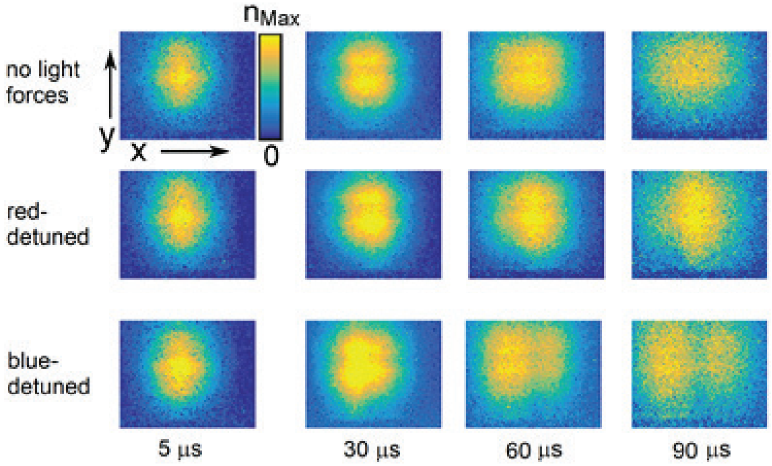

**FIGURE 3.3.1** Laser-induced-fluorescence images of strontium ions in an ultracold neutral plasma. Compared to free evolution (top), lasers red-detuned from the $Sr^+$ principal transition (middle) retard the plasma expansion while they laser-cool the ions. Blue-detuned lasers enhance expansion (bottom). Lasers counterpropagate along the x-axis. SOURCE: Adapted from T.K. Langin, G.M. Gorman, and T.C. Killian, Laser cooling of ions in a neutral plasma, *Science* 363(6422):61-64, 2019, doi: 10.1126/science.aat3158, reprinted with permission from AAAS.

have been seeded in a supersonic molecular beam—for instance, with NO molecules—which explores how molecular processes such as dissociative recombination affect plasma dynamics and the development of spatial correlations.

Ultracold neutral plasmas thus provide another example of how atomic physics techniques can open new, interdisciplinary research directions.

to be the strongest possible, which is the so-called unitary limit in which the scattering length vastly exceeds the typical interparticle spacing. While some significant theoretical understanding of this very challenging regime of many-particle physics has emerged, challenging puzzles remain, and a great deal more needs to be unraveled in future theoretical and experimental studies. See further discussion below in the section "Unitary Quantum Gases."

One major development in the field of ultracold quantum gas physics has been a significant expansion in the types of atoms that can be controlled and brought into quantum degeneracy. In the early days of Bose-Einstein condensation studies, the preferred systems were elements with only one or two valence electrons—namely, the alkali atoms such as rubidium, cesium, sodium, and later hydrogen, metastable helium, ytterbium, and strontium. Within the past decade, it has become possible to treat heavy open-shell atoms as well, such as erbium, dysprosium, and thulium.

Systems of such heavy, open-shell atoms exhibit an incredibly rich array of magnetic resonances that initially looked astonishingly dense, chaotic, and challenging to treat theoretically and to control, but they have turned out to nevertheless enable a surprising degree of quantum control. Enlarging the space of controllable quantum degenerate species has the potential to open wider possibilities of exploration in multiple contexts, such as coexisting multiple spin states, mixed fermionic and bosonic isotopes, strong nonperturbative electric or magnetic dipole-dipole interactions, and anisotropic Van der Waals forces between the atoms. Van der Waals forces are long-range forces between atoms arising from quantum mechanical correlations between the positions of the electrons on different atoms. Such forces occur in many real materials, and their control could prove very fruitful.

The past decade has also seen remarkable growth in theoretical understanding and experimental realizations of polaron physics in dilute atomic gases at very low temperatures. In the ultracold atomic physics context, a polaron is an impurity immersed in, and interacting with, a gas of atoms that are either different species or else the same element but in a different internal spin state. Polaron physics in ultracold atomic systems mimics analogous physics in a number of condensed-matter systems, but with far greater control over the interactions between the impurity and the majority sea of atoms. The committee elaborates on this polaron physics below in the section "Polaron Physics with Ultracold Atoms."

### Unitary Quantum Gases

One of the most interesting topics being studied by experiments and theory 15 years ago was the two-component degenerate Fermi gas, as the atom-atom scattering length $a$ was tuned through the unitary limit, $a \rightarrow$ infinity. The exploration of this regime, denoted the BCS-BEC crossover regime, was notable for showing how the many-body ultracold atomic Fermi gas can be controlled to sweep atoms in a degenerate Fermi gas into diatomic molecules that pair those atoms and form a BEC of molecules. Many remarkable results emerged from those studies, such as the measurement of an accurate equation of state (important for understanding the thermodynamics of such systems) and demonstration of an impressively small rate of destructive molecule-molecule collisions that was partly anticipated by theory and confirmed experimentally.

A next natural step would appear naively to do the same with a BEC formed from bosonic atoms, and similarly sweep the atom-atom scattering length $a$ to this fascinating so-called unitary regime where $a \rightarrow$ infinity. The experimental investigation of the unitary limit of a degenerate Bose gas was resisted for many years, however, largely because three-body recombination losses (due to the process $A + A + A \rightarrow A_2 + A$) have problematic loss rates that scale like $a^4$ and would be catastrophic in the divergent $|a|$ limit. Eventually, however, three-body losses were understood to saturate, and not to diverge at the unitary limit. As a result, in recent years several groups have begun creating Bose gases whose atom-atom interactions are at the unitary limit. In order to minimize losses, these experiments are mostly carried out as "quench experiments," where a stable BEC at small scattering lengths is jumped very quickly to infinite scattering length, followed by a time-dependent response of the quantum gas to this sudden change. In addition to the many-body dynamics that ensue after suddenly changing scattering lengths, highly interesting few-body dynamics also occur, such as turning a fraction of the atoms in the gas into universal dimer and Efimov trimer states. This subject is still in its comparative infancy and remains ripe for extensive future theoretical and experimental investigations.

### Ultracold Gases with Strong Dipole-Dipole Interactions

When the atoms or molecules in a very low temperature system possess a strong electric or magnetic dipole moment, this adds a dominant new element to the possible equilibrium phases that can exist, and to the dynamics that can occur. While no ground-state atom possesses an electric dipole moment, they frequently do possess a magnetic dipole moment. Polar molecules, by definition, possess a permanent electric dipole moment, as do many Rydberg atoms or molecules (see the section below, "Quantum Simulation with Dipolar Interactions"). In contrast to typical van der Waals long-range interactions, which are always attractive for ground-state atoms, dipole-dipole interactions are anisotropic, and have regions of both attraction and repulsion, which makes their resulting few-body and many-body behavior more complicated, but also more interesting (see Figure 3.2). A 3D dipole-interacting system can self-assemble through the mutual attraction into nanodroplets, for instance, connecting with the rich geometrically intriguing behavior of ferrofluids (liquids filled with magnetic particles) studied in condensed-matter physics. On the other hand, if the dipole moments are all parallel and interacting along lines perpendicular to the dipoles in either two-dimensional (2D) pancakes or one-dimensional (1D) rows, the constituent interactions are all mutually repulsive, which can help to suppress undesirable inelastic collision or reactive processes.

Over the past decades, tremendous progress has been made in isolating specific quantum phenomena by focusing on basic systems of coherent light and quantum matter. The acquired knowledge calls now for the next challenge: to explore quantum matter with increasing complexity. Among the different scientific avenues and quantum systems, ultracold quantum gases of highly magnetic atoms constitute one of the most active and promising quantum platforms. A typical quantum gas is composed of about 100,000 atoms. Each of these magnetic atoms can be controlled in their external (motional) and internal (spin) degrees of freedom, and, as a whole many-body system, the particles interact with each other

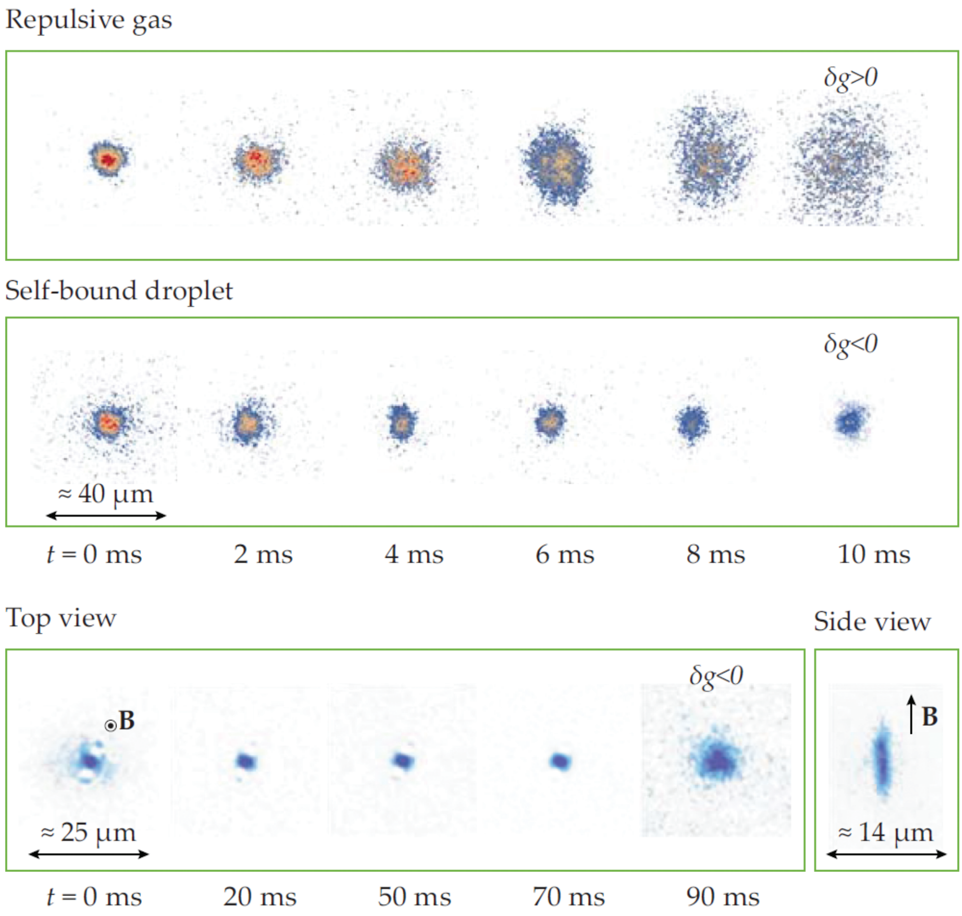

**FIGURE 3.2** Shown are the densities of droplets that can be self-bound in a mixture of two different species of bosonic atoms, each of which has intraspecies repulsion, but with interspecies interactions with a zero-range interaction strength (*g*) that can be tuned from repulsive ($g<0$, top panel) to attractive ($g>0$, bottom two panels). When the mean-field energy of the Bose-Bose mixture is tuned to be repulsive, it produces a gas phase, and the droplet expands as time increases. For the system of magnetic dipolar atoms (erbium atoms, shown in the bottom panel), there are attractive dipole-dipole interactions that can support a regime for the mean-field energy to be attractive, and the size of self-bound droplets stays constant as time increases, although the density gradually decays as a result of three-body loss processes. SOURCE: I. Ferrier-Barbut, Ultradilute quantum droplets, *Physics Today* 72(4):46, 2019, https://doi.org/10.1063/PT.3.4184.

via the ordinary short-range ("contact") and magnetic dipole-dipole interactions. The latter has the key properties of being both long range and anisotropic, and it is expected to result in exciting physics, which is just starting to be unveiled at present. Even the interaction between two heavy open-shell atoms like Er or Dy, which have a huge number of nearly degenerate ground-state energy levels, shows impressive complexity and difficulties for current theoretical methods to understand the atom-atom scattering and resonances.

An extensive amount of new physics can still be discovered and learned from lattice studies, but bulk quantum gases, in which magnetic atoms can move throughout large volumes, have their own mysteries to reveal. Here, novel macroscopic quantum phases of matter emerge, revealing an astonishing universality that connects the behavior of dense quantum fluids (like superfluid helium) to dilute dipolar gases such as those discussed above, through fundamental properties of quantum mechanics. Highlights of recent experimental work with dipolar gases include the observation of macro-droplets, droplet crystals, "roton" excitations analogous to those in superfluid helium, and many-body phases with supersolid properties. The latter is a rather paradoxical quantum phase of matter in which apparently antithetic properties—that is, crystalline solid and superfluid order—coexist. Although intensively searched for in superfluid helium, supersolidity remained a mere theoretical concept for almost five decades, until dipolar gases demonstrated spontaneously emerging states with the regular density patterns of a solid and the global phase coherence of a superfluid.

A major interest over the past two decades of explorations of gas-phase quantum degeneracy has been the study of multiple physical properties of the superfluid. This includes such phenomena as the formation and lifetime of vortices and vortex lattices, collective excitation frequencies, alternative damping mechanisms and sound wave propagation, as well as macroscopic behaviors such as turbulence and granulation. A recent example of granulation can be seen in Figure 3.3. Analogues

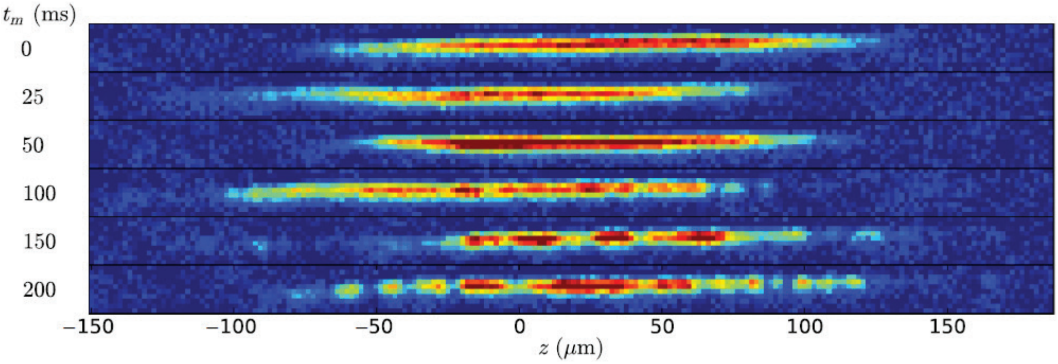

**FIGURE 3.3** Shown is an experimental example of granulation increasing with time. The granulation is created in a Bose-Einstein condensed gas of $^7$Li atoms by modulating the atom-atom interactions at 70 Hz for a time duration $t_m$. SOURCE: J. H.V. Nguyen, M.C. Tsatsos, D. Luo, A.U.J. Lode, G.D. Telles, V.S. Bagnato, and R.G. Hulet, Parametric excitation of a Bose-Einstein condensate: From Faraday waves to granulation, *Physical Review X* 9:011052, 2019, https://doi.org/10.1103/PhysRevX.9.011052, published by the American Physical Society under the terms of the Creative Commons Attribution 4.0 International license.

of classical fluid instabilities such as Taylor-Couette flow or Rayleigh-Bénard convection can also be studied in degenerate quantum gases.

### Polaron Physics with Ultracold Atoms

Ultracold atomic systems have provided us with unique platforms to study the physics of quantum impurities interacting with a medium. The polaron is a quasiparticle that emerges when an impurity atom is coupled to the medium and becomes entangled with ("dressed" by) virtual quantum excitations of the medium. Such quasiparticles represent the cornerstones of most descriptions of many-body systems, as highlighted by Landau's celebrated Fermi-liquid theory, which describes the strongly interacting electron system in terms of a weakly interacting liquid of quasiparticles. While the quasiparticle picture is generally well established, many open questions arise regarding its validity under extreme interaction conditions, or close to phase transitions to ordered states. With an unprecedented level of control, ultracold atomic systems serve as a unique test-bed to address such open questions, to benchmark theoretical descriptions, and to advance our understanding of emergent many-body phenomena.

In a quantum-gas experiment, the medium can have fermionic or bosonic character according to the choice of the particular atomic species. Impurity atoms immersed into the medium then form Fermi polarons or Bose polarons, respectively. To create impurities, one can for instance, excite atoms of the medium into other spin states; alternatively, the system can be doped with another atomic species. Accurate interaction control between the impurity and the medium is a key ingredient, which can be achieved by means of magnetically tuned Feshbach resonances that change the scattering length of the impurity when it interacts with the atoms of the medium. Various experimental tools have been developed to characterize the energy spectrum of the impurities, commonly based on radio-frequency spectroscopic methods. An advanced example is illustrated in Figure 3.4, where a time-domain interferometric method was employed to measure $^{40}$K impurities immersed in a Fermi sea of $^{6}$Li atoms. Various theoretical tools have been developed, including variational methods, functional renormalization group approaches, and descriptions based on functional determinants. Thanks to advances in both experiment and theory, the energy spectrum of polarons is now widely understood in many basic situations, and for large ranges of the interaction strength. It is remarkable, and worth noting, that research on quantum gases has stimulated the discovery of new polaronic quasiparticles in more traditional solid-state semiconductor materials.

New frontiers of polaron physics arise in unexplored regimes, of which three examples are discussed here: (1) Current theoretical understanding of the effect of impurity motion is limited to simple "effective mass" approaches, and almost

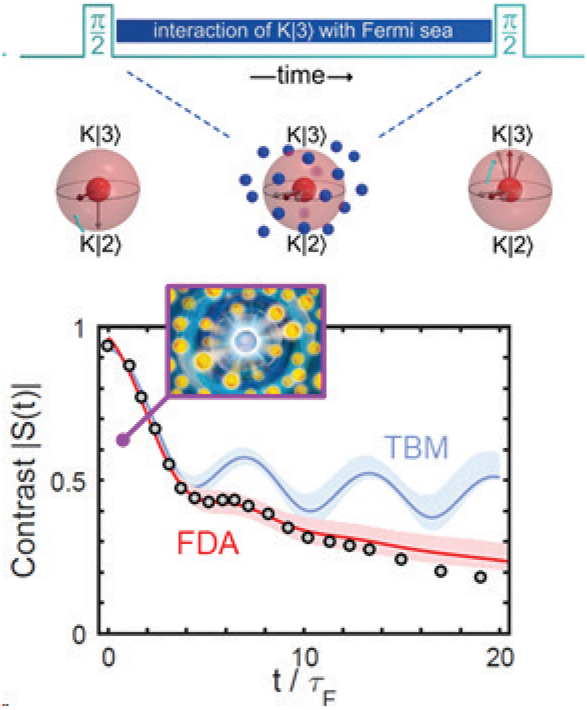

**FIGURE 3.4** Time-domain interferometry on $^{40}$K impurities in a $^{6}$Li Fermi sea (shown as blue dots), and formation dynamics of a repulsive polaron in real time. *Upper panel:* The interferometric scheme consists of a Ramsey sequence of two radio-frequency pi/2-pulses acting on the K impurities (dark red sphere). Between the two pulses, the quasiparticle is in a coherent superposition of an interacting state (K|3>) with a noninteracting state (K|2>). *Lower panel:* The time evolution of the Ramsey contrast signal reveals the formation of the repulsive polaron (the inset shows an artist's view) on the time scale of about four Fermi times ($t_F$ » 3 μs). The experimental results are compared to two different theoretical approaches. NOTE: TBM, truncated basis method, FDA, functional determinant approach. SOURCE: From M. Cetina, M. Jag, R.S. Lous, I. Fritsche, J.T.M. Walraven, R. Grimm, J. Levinsen, M.M. Parish, R. Schmidt, M. Knap, and E. Demler, Ultrafast many-body interferometry of impurities coupled to a Fermi sea, *Science* 354(6308):96-99, 2016, doi: 10.1126/science.aaf5134, reprinted with permission from AAAS.

no experiments have addressed the question of motion so far. The effective mass is a perturbative approach that assumes that the only effect of the medium on the impurity is to increase its apparent mass. This increase in effective mass represents the kinetic energy stored in the atoms of the medium as they "get out of the way" of the moving impurity. The effective mass approximation can be valid only if the quasiparticle motion remains much slower than the characteristic speed (Fermi speed) of the medium. For faster motion, the dressing cloud from the medium can no longer follow the impurity, and a complete breakdown of the quasiparticle picture can be expected. (2) A way to conceptually construct new many-body states is to increase the concentration of polarons up to the point where their mutual interaction leads to new phenomena. While various theoretical predictions have been made for polaron-polaron interactions, experiments so far have shown only a few qualitative effects. Here it will be necessary to carry out new generations of quantitative experiments to test interactions between quasiparticles. (3) Few-body correlations in the medium have been considered theoretically, but in present experiments they have played only minor roles. To explore such correlations, new systems need to be introduced experimentally, such as systems with strong mass imbalance (i.e., consisting of different types of atoms with different masses), which provide access to new phenomena.

Polaron physics with ultracold atoms provides paradigmatic situations to approach many-body behavior. In future research, it will be important to complete our understanding on the emergence of many-body phenomena and to learn more about the connection to ordered states, such as novel superfluids. In a cross-disciplinary sense, it will be very fruitful to further build on the analogies of AMO-based systems with real condensed-matter systems.

## MANY-BODY SYSTEMS WITH ULTRACOLD MOLECULES

In comparison with atoms, molecules have a much more complex level structure and many more quantum degrees of freedom, and their control is a major challenge in achieving ultracold molecular quantum gases. At the same time, the complexity of molecular systems provides new opportunities for engineering quantum many-body systems beyond the atomic counterparts. (See, for example, "Introduction to Ultracold Molecules: New Frontiers in Quantum and Chemical Physics," *Chemical Reviews*, Volume 112, Issue 9 (Special Issue), September 12, 2012.)

### Cooling and Trapping Molecules for Complete Quantum Control

Trapping and cooling of atoms are core techniques in atomic physics. Trapping provides time to measure and manipulate atoms with exquisite precision, while cooling reduces disorder in the system, and hence increases the certainty that the system starts in a specific, defined quantum state. As systems become larger and more complex, the number of possible states increases rapidly, and cooling to achieve complete quantum control becomes more important—but also more difficult.

Systems made of molecules rather than atoms have more potential to become complex. In addition to their overall motion, molecules have a richer internal structure that includes vibrations and rotations. Under sufficient control, these internal states can be used as a powerful quantum resource—particularly when the overall motion is also cooled and the molecules are trapped. For example, the rotational structure of polar molecules can be used to amplify tiny energy-level shifts, indicating the existence of as-yet undiscovered fundamental particles—or, instead, to engineer tunable, long-range dipolar interactions between trapped molecules, with potential applications in quantum simulation and quantum information processing. The diversity of molecular species also opens the door to study of chemical processes; at ultracold temperatures, novel quantum effects can appear in chemical reaction dynamics.

These promising applications have motivated intense efforts to bring molecules under complete quantum control. Despite the challenges associated with controlling their complex internal structure, progress has been very rapid. In one of two primary methods, diatomic molecules are assembled from ultracold, trapped precursor atoms. This approach yields exceptionally low temperatures; it has enabled trapping of molecular arrays in optical lattices, and production of a quantum-degenerate gas of polar molecules. The range of molecular species that can be assembled in this way is limited, but sufficient for some envisioned applications.

In the meantime, methods for direct laser cooling and trapping of molecules also have been developed. This approach uses techniques similar to those now standard for atoms, and yields similar results. For example, laser-cooled molecules have been accumulated in magneto-optical traps, then transferred at ultracold temperature to dipole traps or tweezers—as needed for further cooling. This approach is proving applicable even to polyatomic molecules. Although not yet as advanced as the method of ultracold molecule assembly, laser cooling is proving far more general, and its outcomes are improving rapidly (see Figure 3.5).

Techniques for preparing ultracold molecules are new and rapidly improving, and their application promises a wide range of important science in the coming decade. As is discussed later in this chapter, it seems likely that molecules in optical lattices will be used to probe—and possibly detect—new fundamental physics, at energy scales far beyond those accessible with high-energy particle colliders. Physics at ultrahigh energy scales is accessible in table-top experiments through the extreme precision of AMO techniques, which can detect the tiny effects of high-energy phenomena on low-energy quantum states of atoms and molecules. Similar experiments can perform quantum simulations of highly correlated many-body systems such as spin lattice Hamiltonians with topological phases. Arrays of individual molecules in reconfigurable optical tweezer arrays may provide deterministic preparation of many-body systems along with high-fidelity detection, potentially opening new avenues in quantum computing and simulation. (See Chapter 4 for further discussion.)

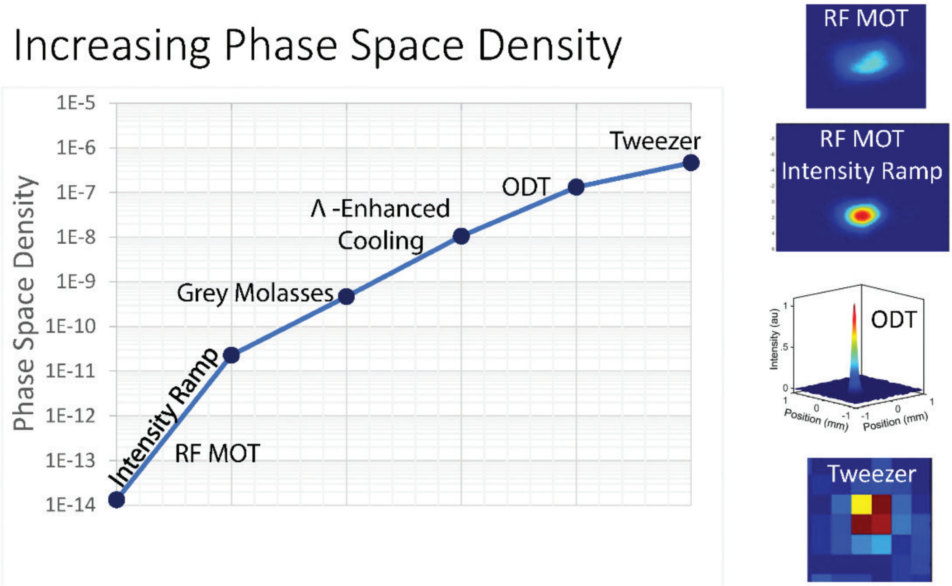

**FIGURE 3.5** Direct laser cooling and trapping of molecules. The plot shows phase-space density—a quantity whose increase corresponds to a decrease of disorder—in a sample of laser-cooled and trapped calcium monofluoride (CaF) molecules, at various stages of an experiment. Increasing the phase space density by nearly eight orders of magnitude requires multiple experimental stages using distinct techniques. At the highest density, the final step is an array of CaF molecules trapped in optical tweezers, an arrangement that has potential for use as a qubit platform. NOTE: ODT, optical dipole traps. SOURCE: Courtesy of John Doyle, Harvard University.

### Many-Body Systems Based on Ultracold Molecules

Samples of optically trapped ultracold polar molecules can now be produced in many laboratories. One of the most compelling applications for these molecules is to use them as elements in future programmable quantum simulators. In particular, the molecule frame electric dipole moment ordinarily rotates in the laboratory frame at microwave-scale (or lower) frequencies with a very long lifetime, making it natural to encode quantum information in this degree of freedom. The interaction between molecular electric dipoles is strong and long-ranged. Hence, even when molecules are separated by distances on the order of the wavelength of visible light, this coupling between molecules may dominate the dynamics of the system. This means that many-body systems of polar molecules in optical lattices or tweezer arrays can be engineered to become highly entangled, and to remain so for long times.

Many pioneering advances in this direction have been made in experiments using KRb molecules—for example, in the laboratories of Deborah Jin and Jun Ye at JILA. Here, out of K and Rb ultracold atoms loaded into a common optical dipole trap, the JILA team assembled fermionic KRb molecules at a temperature of ~200 nK. These molecules are produced in the electronic-vibrational-rotational-hyperfine ground state, and a degenerate Fermi gas of molecules is born with a temperature just 30 percent of the Fermi temperature. These molecules have also been loaded in a 3D optical lattice, achieving a lattice filling of ~25 percent for ground-state KRb molecules. This is of the order of the "percolation threshold" in 3D, and surpasses it when as here every molecule is connected to all others via electric dipole-dipole interactions (see Figure 3.6). This team also simulated a direct, long-range spin-exchange coupling between two ground-state KRb molecules by encoding an effective spin into a pair of rotational states with dipolar interactions. This allowed observation of many-body spin dynamics with the spin and motional degrees of freedom completely decoupled.

In the meantime, ultracold molecule systems based on several other bi-alkali species have been developed in other laboratories around the world. For example, some new experiments use molecules that have much larger dipole moments, enabling stronger interactions. In some cases, these species, unlike KRb, cannot chemically react with each other; this mitigates losses while preparing the molecular samples. These and other experiments have demonstrated long coherence times of molecular spin superpositions, and improved rotational state coherence by better optimizing the optical-lattice parameters. These constitute early, but extremely promising first steps toward using ultracold polar molecules as a system for interesting, novel types of quantum simulations, as discussed below.

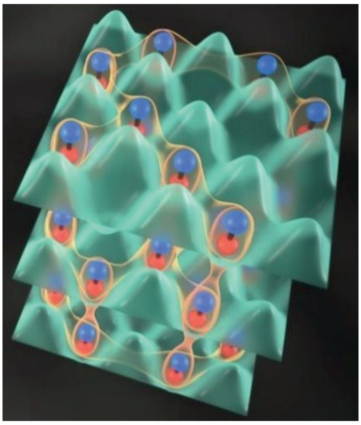

**FIGURE 3.6** Ultracold polar molecules in a three-dimensional optical lattice. With a sufficiently large fraction of sites filled, long-range electric dipole-dipole interactions are strong enough to ensure that each molecule is effectively coupled to all others in the lattice. SOURCE: National Institute of Standards and Technology, "It's a Beauty: JILA's Quantum Crystal is Now More Valuable," News, November 5, 2015, https://www.nist.gov/news-events/news/2015/11/its-beauty-jilas-quantum-crystal-now-more-valuable.

## ANALOG QUANTUM SIMULATION OF STRONGLY CORRELATED QUANTUM MANY-BODY SYSTEMS

A typical BEC represents a weakly interacting many-body system, where a mean-field (average interaction) description is often sufficient to describe the underlying physics. In contrast, one of the fundamental challenges of quantum science is to understand the strongly correlated quantum many-body regimes where mean-field theory breaks down. These regimes generally have large critical fluctuations. Quantum phase transitions (for example, believed to underlie high-temperature superconductivity) are of particular interest. These sorts of many-body systems define one of the present frontiers of theoretical condensed-matter physics for both equilibrium and non-equilibrium phenomena. Such a strongly correlated many-body system can be built, for example, by loading a BEC or a degenerate Fermi gas into an optical lattice—that is, into a periodic array of microtraps generated by counterpropagating off-resonant laser light fields, with a lattice spacing given by half the wavelength of the light.

Atoms loaded into an optical lattice can hop between lattice sites via tunneling processes, reminiscent of electrons moving in a crystal lattice of solid-state physics, and these atoms interact with each other through molecular forces. Such atoms loaded into an optical lattice acquire an effective mass, which is tunable with the strength of the laser intensity defining the lattice structure, and can be much larger than the free-space mass. Another way to look at this is to note that the tunneling between neighbors can be enhanced or suppressed by lowering or raising the light intensity field forming the barriers between lattice sites. This provides control over "kinetic" versus (on-site) "interaction" energies, and thus allows one to tune these systems from weakly to strongly interacting. This particular system enables the realization of the Bose-Hubbard and Fermi-Hubbard models of condensed-matter physics—namely, the Hubbard model with bosonic or fermionic atomic or molecular components. Moreover, it opens the door toward realizing strongly correlated quantum phases in a laboratory setting, by tuning of the Hubbard parameters via external fields. Hubbard models built from ultracold atoms and molecules in an optical lattice provide us with a paradigmatic example of an "analog quantum simulator," where a quantum many-body system can be realized in a controlled setting. The unique possibility of controlling AMO systems via electromagnetic (static, optical, and microwave) fields provides us with a toolbox, with which numerous many-body Hamiltonians of interest can be designed. These include models of superconductivity, of ferromagnetism and anti-ferromagnetism, of spin glasses and spin liquids, of Anderson and of many-body localization, and of complex competing phases including topological ones. Recent examples of extending the range of Hamiltonians that can be simulated include synthetic magnetic fields (or synthetic gauge fields, which can mimic magnetic fields or other types of force fields), or long-range interactions provided by dipolar interactions from magnetic or electric dipoles, and of various forms of disorder. Engineering many-body Hamiltonians within a given set of control knobs is, of course, just one facet of simulating quantum many-body physics with atoms and molecules. Additional key elements are protocols for preparation of quantum phases, or initial states. Furthermore, atomic and molecular physics provides unique abilities to measure many-body observables and correlation functions: a seminal example is the quantum gas microscope for optical lattices, which allows single-site, particle- and spin-resolved readout in single-shot measurements.

While most of our discussion below will focus on analog quantum simulators as emulating the dynamics of an isolated quantum many-body system in equilibrium and non-equilibrium dynamics, one can extend this notion to treat an open system as well, where the coupling to a bath is designed by quantum reservoir engineering. This includes in particular driven-dissipative systems, where the many-body system approaches a dynamical equilibrium, with the potential to observe new non-equilibrium phases and phase transitions. In addition, this can be developed into a tool for preparing interesting entangled states, as relevant for quantum information applications (see Chapter 4). Such simulations give deep insight into the role of entanglement in quantum thermalization (as discussed further in Chapter 7).

### Quantum Simulation of Fermi-Hubbard Models in Various Spatial Dimensions

As described above, quantum simulation of the Hubbard model with ultracold fermionic atoms in optical lattices is a prime example of emerging quantum systems. Study of this particular Hamiltonian enables AMO physicists to address crucial open questions in many-body quantum mechanics and materials science. This iconic model is, at the same time, both computationally extremely challenging and highly relevant. It is believed to capture the essential physics of high-temperature superconductors and other quantum materials; however, no first principles understanding of this "deceivingly" simple model exists. Hence, in the upcoming years, quantum simulations have the potential to exert a large impact on the understanding of this physics, and potentially to help us design new high-temperature superconductors.

Recent experiments, in which fermionic atoms in optical lattices mimic electrons hopping in a crystal lattice, are a virtually perfect realization of the Hubbard model (see Figure 3.7). Quantum gas microscopy enables ultimate control for readout and manipulation, on a single-site, single-atom level. Parameters can be widely tuned, and with the observation of anti-ferromagnetism, experiments are now starting to explore the low-temperature phases of the model. Doping away from half filling brings the system into poorly understood terrain, and phases such as strange metals, pseudogap phases, and the important high-temperature superconducting phase are hoped to be seen. The complexity of these phases stems from the intricate

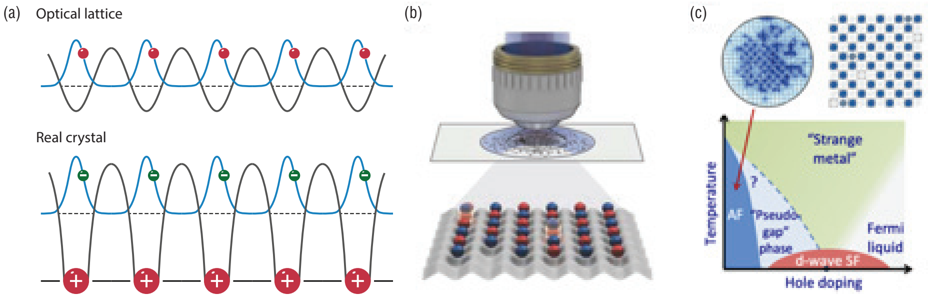

FIGURE 3.7 (a) Ultracold fermionic atoms in an optical lattice form a model system for simulating strongly correlated electron systems in materials. (b) Quantum gas microscopy enables ultimate microscopic control for detection and manipulation. (c) Experiments are now starting to realize low-temperature phases of the iconic Hubbard model (image: quantum gas microscope snapshot of a Fermi-Hubbard antiferromagnet). This model is believed to capture the physics of the strange metal, pseudogap, and high-temperature superconducting phases. Currently, there is no unified understanding of these phases, and computations for the Hubbard model are extremely challenging. In the next years, it is expected that quantum simulations will play an important role in exploring this and similar models, with potential large impact on quantum materials and beyond. SOURCE: Courtesy of Markus Greiner, Harvard University; panels b and c adapted by permission from Springer Nature: A. Mazurenko, C.S. Chiu, G. Ji, M.F. Parsons, M. Kanász-Nagy, R. Schmidt, F. Grusdt, E. Demler, D. Greif, and M. Greiner, A cold-atom Fermi–Hubbard antiferromagnet, *Nature* 545:462-466, 2017, doi:10.1038/nature22362, copyright 2017.

interplay between spin and charge degrees of freedom, and the fermionic nature of the particles. Experiments have started to explore the doped Hubbard model, probing string-like excitations and allowing theories to be benchmarked. Particularly useful are experiments on transport and non-equilibrium physics, which are doubly hard numerically. Recent experiments, for example, study transport in the doped regime, where measuring resistivity that varies linearly with temperature is the hallmark for strange metal behavior. Other experiments directly observe the microscopic motion of holes in the antiferromagnetic environment.

The recent experimental breakthroughs in fermionic quantum simulation, in which experiments are demonstrating a genuine quantum advantage over simulations on classical computers in particular in 2D and 3D, provide a unique opportunity for discovery during the coming years. Among the key challenges is measurement of the complete phase diagram of the 2D Hubbard model with repulsive onsite interactions, as a paradigmatic model for high critical temperature ($T_c$) superconductivity; this is a problem for which computational complexity provides a fundamental limitation to fermionic quantum Monte Carlo simulations. Quantum gas microscopy plays a particularly important role in this. It enables experimenters to take a complete quantum "snapshot" of a complex strongly correlated many-body quantum state, which is unprecedented in physics. This capability is complementary to the kind of observables available in condensed-matter physics. Snapshots enable the direct detection of patterns and of high-order multiparticle correlation functions. This gives the possibility to find "hidden order," which can even be facilitated by machine learning. By measuring correlations between the motion of charge carriers, and simultaneously registering microscopic fluctuations in the surrounding magnetic environment, it may be possible to answer open questions concerning the nature of the superconducting pairing mechanism in the Hubbard model, and to shed light onto the pseudogap regime. At temperatures a few times lower than currently achieved, Cooper pairs may form a superfluid phase, which is a likely analogue of the superconducting phase in high-temperature superconductors. A key goal will be to answer outstanding questions, such as whether the superconducting phase is competing with, or emerging from, the antiferromagnetic phase.

Will such simulation of the Hubbard model hold the key to high-temperature superconductivity? There are many reasons to believe that the plain Hubbard model contains most—but not all—of the ingredients necessary for understanding high-temperature superconductivity in the cuprates. A full explanation is likely to require additional ingredients in the model although there is no consensus about which, if any, are important. But that is just where the remarkable control over ultracold atoms in an optical lattice comes into its own—the idea is to approach the problem by realizing the bare Hubbard model first and then adding other ingredients, as needed, in a controlled way.

By adding additional terms to the 2D fermionic Hubbard Hamiltonian—for example, offsite interactions, long-range hoppings or synthetic gauge fields, or by simply changing the lattice geometry, quantum simulation of a broad range of phenomena could be enabled. Further expanding the Hamiltonian will help shed light on other open questions such as frustrated quantum magnets, topological phases, spin glasses and spin liquids, localization, as well as provide new insight into non-equilibrium physics. Such phases will be uniquely realized and studied with fermions in optical lattices, while quantum gas microscopy provides detection ("state tomography") on a genuinely many-body quantum level.

### Quantum Simulation with Dipolar Interactions

Dipolar interactions provide anisotropic and long-range couplings between particles, as compared to short-range contact potentials. In the toolbox of quantum simulation, this provides new elements to engineer and explore long-range interactions. There is a rich literature of theoretical proposals for how to engineer strongly correlated quantum many-body systems with ultracold magnetic atoms and ultracold polar molecules, and these phenomena are now beginning to be explored in the laboratory, both with highly magnetic atoms in optical lattices (such as chromium, dysprosium, and erbium) and with polar molecules where electric dipole moments can provide even stronger dipolar couplings.

For magnetic atoms, recent experimental highlights include both the realization of extended Bose-Hubbard models and spin lattice models, in which the superfluid-to-Mott-insulator phase transition and the spin dynamics are largely determined by the dipolar coupling between particles occupying different lattice sites (see Figure 3.8).

The unique feature of polar molecules in designing quantum simulators is, first of all, their strong electric dipoles and corresponding strong dipolar interactions. In addition, molecules offer new methods for control—for example, microwave dressing to couple rotational states to internal spin states, and further cooling for reduced ensemble entropy—that will likely bring to fruition many of the theoretical ideas around the paradigm of dipolar interactions. Some proposed examples include observing a novel self-stabilized crystalline phase, simulating nontrivial quantum magnets, producing symmetry-protected topological phases or phases with true topological order such as fractional Chern insulators, and so on. In additional to polar molecules and dipolar atoms, many-body quantum dynamics of dipolar systems are also being explored with programmable Rydberg simulators and spin defects in diamond, as discussed in Chapter 4. These developments represent a broad new frontier in quantum science.

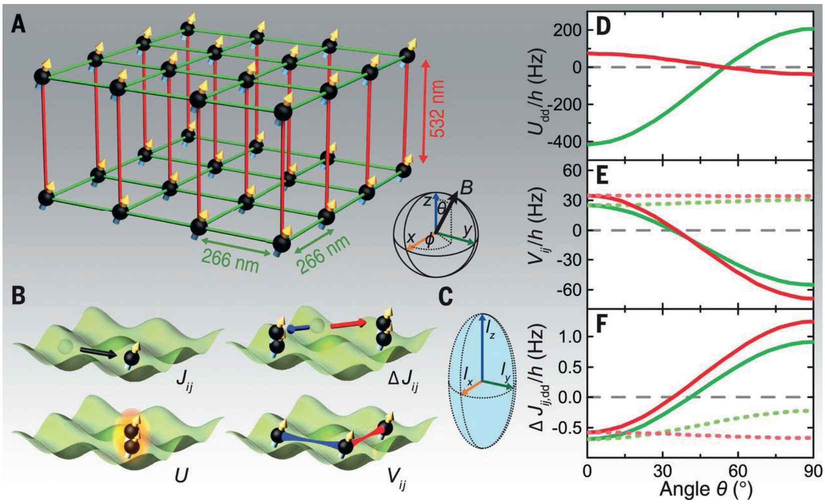

**FIGURE 3.8** *Left:* Dipolar atoms in a 3D crystal of light, realizing an extended Bose-Hubbard model. *Right:* Tunneling ($J$) and interaction terms ($U$ and $V$), including off-site terms. SOURCE: From S. Baier, M.J. Mark, D. Petter, K. Aikawa, L. Chomaz, Z. Cai, M. Baranov, P. Zoller, and F. Ferlaino, Extended Bose-Hubbard models with ultracold magnetic atoms, *Science* 352(6282):201-205, 2016, doi:10.1126/science.aac9812, reprinted with permission from AAAS.

## Artificially Engineered Gauge Potentials

One of the unexpected developments during the past decade has been a strong growth in the field of spin-orbit coupled quantum gases. Whereas the coupling between the orbital and spin magnetic moments of atomic electrons has been studied in atomic spectroscopy for more than a century, a very different type of spin-orbit coupling (SOC) can be created for an atom in a laser field. In this situation, the intrinsic spin degrees of freedom are coupled to the linear momentum of the atom. This has been demonstrated experimentally by many groups already, and it connects with studies of so-called Rashba or Dresselhaus spin-orbit coupling that arises extensively for electrons in condensed matter. The use of lasers to drive Raman transitions can also engineer unusual dispersion relations such as linear Dirac cones in the momentum dependence of the atomic energy landscape. Interestingly, such a Dirac cone provides a way to mimic or simulate the fundamental high-energy quantum mechanical equation (Dirac equation) in a low-energy system. This opens up connections with the physics of topological band structures of tremendous current interest in condensed-matter physics. This line of research with spin-orbit coupling in atomic gases has added significantly to our ability to controllably simulate emerging and challenging phenomena in condensed-matter physics using ultracold atomic systems.

Another recent creative growth area for the field of ultracold atomic systems has been the introduction of techniques to create a "synthetic dimension." Typically, cold quantum gases are designed to exist in a 3D trap, or in some cases in reduced dimensional traps—for example, of a pancake-type 2D geometry or a cigar-shaped 1D geometry. The idea of a synthetic dimension arises when one couples the atomic states into a spin degree of freedom with several states that behave very analogously to a true spatial dimension. Consider for example an atom moving in one dimension by hopping (tunneling) between adjacent wells of a cigar-shaped optical lattice. If the atom has, say, five distinct internal spin states, one can arrange for hopping transitions to occur among the neighboring spin states in such a way that the atom appears to be moving in quasi-2D optical lattice strip of width 5. Quantum gas systems with a synthetic dimension have been used to explore a version of the famous quantum Hall effect in condensed-matter systems, except that in the cold atom version of this effect, the motion of electrically neutral atoms mimics the behavior of charged electrons in a strong magnetic field.

The unique properties of alkaline-earth atoms and recently developed precision clock-spectroscopy capabilities make such cold atom systems an ideal platform to engineer and study exotic forms of quantum matter—ideal because of the extensive controllability of the relevant parameter spaces involved. For example, fermionic $^{87}$Sr atoms can be prepared in long-lived $^1S_0$ and $^3P_0$ electronic orbitals, each with 10 nuclear spin sublevels ($^{87}$Sr has nuclear spin $I = 9/2$), and trapped in an optical lattice with 1D, 2D, or 3D geometries. For example, in a 3D lattice with the Sr gas cold enough to be Fermi degenerate, all degrees of freedom, including the electronic, nuclear, and motional quantum states, are fully controlled, and the resulting few- to many-body properties and dynamics can be probed with extremely high precision—that is, with sub-Hertz spectral resolution.

Theoretical investigations of correlated quantum many-body systems have proceeded at an astonishing pace. However, experimental progress on such correlated systems embodied in atomic quantum gases has been hampered by the extremely low entropy (essentially temperature) required to observe novel quantum phases. A complementary approach to study some of these phenomena is to focus instead on the non-equilibrium many-body spin dynamics. This allows precise investigations and observations of intrinsic signatures for collective spin interactions, including strongly modified spectral shapes, spin dephasing and decoherence, interaction-induced frequency shifts, and correlated quantum spin noise. Describing these observations requires a genuine many-body theory reaching beyond the conventional mean-field framework.

Another surprising development is the use of the tremendous precision of optical lattice clocks to study an important topic in many-body physics—spin symmetry and its effect on many-body phenomena. In alkaline-earth atoms, the nuclear spin can be in $N$ distinct states, which makes atoms in different states distinguishable in principle. However, because the electrons have total spin and orbital angular momentum $J = 0$, the nuclei in the interior of the atoms have no effect on the exterior shell of electrons. Thus, the atom-atom interactions (determined by the electrons) are almost completely independent of the nuclear states. This special symmetry of the atom interactions (known as $SU[N]$ symmetry) leads to novel many-body effects. When $N$ nuclear-spin sublevels are populated in this system, one can directly and precisely probe atomic interactions under the $SU(N)$ symmetry. Recent clock spectroscopy results provided the first direct observation of $SU(N)$ symmetry for alkaline-earth atoms and the related two-orbital $SU(N)$ magnetism. Non-equilibrium spin-orbital dynamics in $SU(N)$ magnetism was directly measured (for $N \leq 10$) via Ramsey spectroscopy. The unique approach enabled by the exquisite energy resolution of optical lattice clocks paves the way for future exploration of the fascinating consequences of $SU(N)$ symmetry in spin-orbital lattice models, as well as test-beds for high-energy lattice gauge theories.

By allowing the atoms to tunnel in an optical lattice, exotic new phenomena governed by the competition between interactions and correlated spin motion can be probed. A single neutral Sr atom tunneling in the lattice, when interrogated by the clock laser, can behave as a charged electron moving in an ultrastrong magnetic field. This synthetic field arises from a simple act of having the clock laser imprint a local quantum phase that varies from one lattice site to the next. Hence, when an atom traverses a closed loop, it accumulates a net phase as if it were a charge that was encircling magnetic flux. The effect of the laser on the atom can also be arranged to generate a coupling between the atomic motion and internal states—that is, SOC—as every time an atom changes its internal level by absorbing or emitting a photon, it experiences a momentum kick. With a quantum-degenerate $^{87}$Sr Fermi gas loaded into a 3D optical lattice, clock spectroscopy can directly probe SOC in higher dimensions. The system can be modeled using few- and many-body approaches; these studies seek new physics induced by the interplay between SOC and interactions such as those that occur in topological superfluids, which host protected Majorana modes, a vehicle of interest for topologically protected quantum computation.

### Topological Matter with Cold Atoms

Topology is the field of mathematics that studies the most fundamental properties associated with the shapes of objects—namely, those properties that do not change when the object is continuously deformed. The number of holes in an object is one example of a topological invariant. Thus, a donut and a coffee cup, although they look quite different, can be continuously deformed into each other because they both have one hole. In recent decades, topology has been discovered to lie at the heart of many striking physical phenomena, ranging from topological defects (e.g., magnetic monopoles and vortices) to topological states of matter. These phenomena are robust, here not against changes in the shape of the sample, but rather against smooth deformations of the geometry of the quantum states themselves. This in turn implies that the phenomena are robust under continuous deformations (or errors) in the values of the parameters describing the energy and interactions of the particles in the system. Since their discovery in the solid state, topological states have attracted the interest of a wide scientific community for their unusual transport properties, suggesting promising technological applications. For example, one can readily imagine spintronics-based devices that are robust against small errors in device fabrication. In addition, certain classes of topological states host exotic excitations (so-called non-Abelian anyons), which, if properly manipulated, could be used as building blocks for fault-tolerant quantum computations. Today, in parallel to the intense effort that is dedicated to the search for novel topological materials, a substantial research activity concerns the realization of topological states using engineered quantum systems, such as ultracold gases trapped in optical lattices. Indeed, these engineered systems could offer the possibility of accessing a wide variety of topological phenomena in a highly controllable environment, an ideal setting to explore and manipulate topological matter in regimes that are hardly accessible in the solid state.

Major steps have been achieved in the past decade in terms of creating topological states of matter in ultracold gases. The first topological phenomena have recently been reported by several experimental groups worldwide. These achievements concern the realization of topological energy level structures (so-called "Bloch bands") for neutral atoms, which can be designed through artificial magnetic fields and spin-orbit couplings (as described in the previous section). Also of interest are the development of novel probes for geometric and topological band properties, which can, for instance, enable assessments of the robustness of the topological protection of various quantum mechanical states against decoherence. Within the past 5 years, this progress led to the measurement of the topologically invariant Chern number of Bloch bands, to the extraction of the local Berry curvature, and to the realization of topological pumps in atomic gases. Very recently, ultracold gases revealed novel topological effects; these include the observation of topological Anderson insulators in the presence of engineered disorder, the detection of higher order Chern numbers, and the observation of quantized circular dichroism. Such phenomena are at least for now inaccessible in traditional materials. Such topological phenomena are important in condensed-matter systems such as the fractional quantum Hall effect, and the advantage of realizing them with ultracold gases is that they can now be probed and controlled in exquisite detail by realizing them in a system of laser-trapped atoms.

Cold-atom experiments exploring topological phenomena are currently restricted to operating in the noninteracting (or weakly interacting) regime, where the properties of interest can be deduced from single-particle band structures. The strongly correlated regime of topological matter could be reached by enhancing the interactions between the atoms, which can be easily achieved in these setups. However, current experiments have shown that severe heating and instability mechanisms result when combining the techniques that are used to generate the topological band structures (i.e., artificial gauge fields) with strong interactions. As a result, a major challenge today concerns the elimination of heating processes and the stabilization of strongly interacting atomic gases in the presence of artificial gauge fields. An interesting route toward this goal involves the preparation of target topological states through engineered dissipation. Once stabilized in the laboratory, it will be crucial to develop proper probing schemes to detect the intriguing properties of these interacting topological states. A significant question concerns the detection of non-Abelian anyons (such as individual zero modes of Majorana—and Majorana fermions formed by pairs of such zero modes) in this atomic context. This would be an important step toward exploration of new science, and such phenomena are also believed to hold promise for technologically important applications in quantum information processing.

The realization of strongly correlated topological states of matter using ultracold atomic gases is deeply connected to another active field of research: the quantum simulation of lattice gauge theories, for probing fundamental particle physics. Not only are topology and lattice gauge theories deeply related at the theoretical level, the proposed schemes to realize dynamical gauge fields (and the required matter-gauge field couplings) in the laboratory are reminiscent of those currently exploited to create topological band structures. First, experimental achievements along these lines include the cold-atom implementation of a minimal toric-code Hamiltonian, as well as the engineering of density-dependent gauge fields leading to a minimal Z2 lattice gauge theory. These developments suggest that intense pluridisciplinary activities can be expected in the next few years, hence further connecting the condensed-matter, high-energy, and quantum optics (AMO physics) communities. The report will return to quantum simulation of dynamical gauge fields—that is, where the gauge field becomes a dynamical variable—in Chapter 4.

### Non-Equilibrium Quantum Many-Body Dynamics

Understanding the non-equilibrium dynamics of strongly interacting quantum systems represents a central challenge that connects AMO physics to a number of other disciplines including condensed-matter, high-energy, and quantum information science. This challenge stems in part from the fact that quantum systems can be taken out of equilibrium in a multitude of different ways, each with its own set of expectations and guiding intuition. The various strategies for exploring non-equilibrium quantum physics might be broadly summarized into six categories:

1. Quench initial conditions;
2. Periodic (Floquet) driving;
3. Strong disorder leading to the breakdown of statistical mechanics (this phenomenon is related to the effect that is sometimes referred to as "many-body localization (MBL)");
4. Dissipative coupling to an environment;
5. Critically slow dynamics; and
6. Prethermalization.
7. Quantum- and nano-thermodyanmics

The diversity of expectations from each of these different microscopic scenarios is readily apparent. For example, under a sudden quench (controlled change of system parameters), one typically expects a many-body system to quickly evolve toward a new local thermal equilibrium. At first sight, this suggests a simple description. However, capturing both the microscopic details of short-time thermalization as well as the crossover to late-time hydrodynamics (in which the local density of quantities protected by conservation laws relax very slowly) remains extremely difficult. Alternatively, a many-body system can also be taken out of equilibrium via Floquet driving (via periodic modulation of external control parameters in the system). In this case, the non-equilibrium system is generically expected to absorb energy from the driving field (although in some cases it may temporarily achieve pseudo-equilibrium on short time scales).

Some of the most unique and stunning physical phenomena sit precisely at the interface between these various non-equilibrium strategies; these include, for example, questions regarding fundamental speed limits on the propagation of quantum information as well as the dissipative stabilization of entanglement and localized quantum memories.

Perhaps one of the most surprising insights to come out of the study of non-equilibrium AMO systems this past decade is the discovery of new phases of intrinsically non-equilibrium quantum matter. Indeed, previous classifications of matter relied on thermodynamic equilibrium. In particular, from the viewpoint of many-body physics, all phases of matter should satisfy certain properties that embody the notion of rigidity. First, the system should have many locally coupled degrees of freedom so that a notion of spatial dimension and thermodynamic limit can be defined. Second, within a well-defined thermodynamic phase, the system's ordering should be robust against a wide range of perturbations of both the initial state and the equations of motion.

These topics are currently being explored in a wide variety of AMO systems, including ultracold gases in a quantum simulator setting and trapped-ion analog quantum simulators (see also Chapter 4). Below, the committee discusses how the techniques of quantum gas microscopy are being used to experimentally study many-body localization—a very active topic in many-body physics. Quantum entanglement also plays a key role in non-equilibrium dynamics, and is discussed in the following chapters.

### Observation of Many-Body Localization

Far from equilibrium, settings pose some of the most challenging and complex problems in quantum many-body physics. They often involve a rapid and extensive growth of entanglement in the quantum system, making it quickly intractable to an attempted numerical simulation on modern classical supercomputers. Nevertheless, these settings pose fundamental open questions concerning the emergence of thermalization in closed quantum systems, transport properties, and the susceptibility of these systems to classical noise or driving. In equilibrium thermodynamics, one assumes the existence of an infinitely large "bath" that can exchange energy (and in some cases particles) with the system under study. Weak interactions with the bath bring the system into equilibrium at the same temperature as the bath. In contrast, atomic systems can be nearly perfectly isolated from the environment—for example, sub-microKelvin temperatures are routinely achieved via laser cooling in an apparatus sitting at room temperature. For an isolated system, the particle number and total energy are fixed, and the only "bath" the particles see

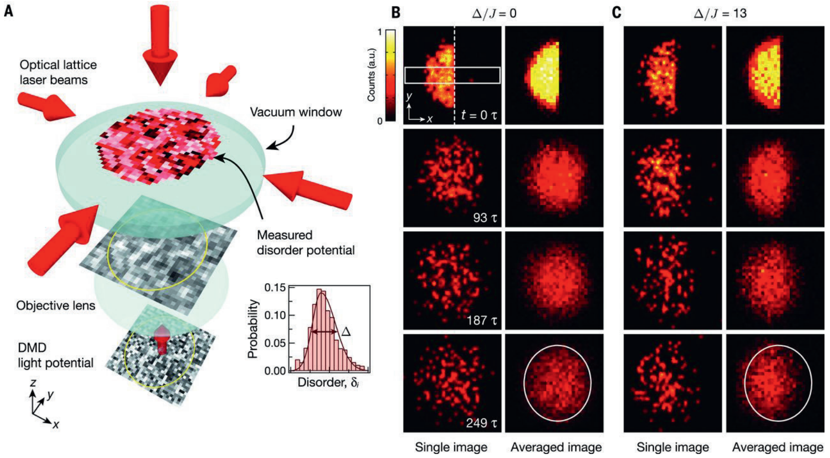

**FIGURE 3.9** Probing many-body localization in two dimensions with a quantum gas microscope. The left part of the figure schematically shows the generation of the random optical disorder, which is projected onto the atoms in the optical lattice using a high resolution objective. The series of images on the right show microscopic images of the system resolving individual atoms by their localized fluorescence. Comparing the average images on the bottom right (those containing the white circle), localization becomes apparent by the missing atomic density in the right half of the white circle (lower right item). A. Huse, I. Bloch, and C. Gross, Exploring the many-body localization transition in two dimensions, *Science* 52(6293):1547-1552, 2016, doi:10.1126/science.aaf8834, reprinted with permission from AAAS. Caption provided by corresponding author Dr. Christian Gross.

are each other. How (and if) such a closed quantum system reaches equilibrium following a sudden quench of parameters is an exciting research frontier at present. These questions are also deeply linked to emerging quantum technologies, whose protocols involve dynamical control of quantum many-body systems in one way or another. Analog AMO quantum simulators can provide experimental insight into these fundamental and challenging problems (see Figure 3.9).

One of the most prominent topics in this context is the question of if and how localization and non-ergodicity can emerge in a generic interacting many-body setting. Such very unfamiliar nonthermal behavior is called "many-body localization (MBL)," a phenomenon in which long-range transport of extensive quantities (e.g., energy or particles) is absent, and quantum properties of the macroscopically large system can be preserved over very long times.

The theoretical treatment of localization phenomena in quantum systems dates back to the 1950s, when Anderson wrote his celebrated article about localization of electrons in disordered lattices. It took many years until the effect of interactions could be added into this picture, with Mott for example early on finding localization in an interacting but not disordered metal; and only in 2006, based on new theoretical results, has localization been predicted to emerge in a disordered and interacting system, at finite-energy densities and in one dimension. (The stability of the localized phase in higher dimensions has not been firmly established.) This defined the notion of MBL, and triggered many theoretical works aimed to understand the mechanisms and implications of localization, the dynamical and static properties of the localized phase, the nature of the phase transition between the ergodic and localized phases, and many more aspects of this novel stable nonthermal phase of quantum matter. Interestingly, and perhaps not surprisingly due to the fact that MBL is a true quantum phenomenon, it has turned out that quantum information theoretical concepts such as entanglement entropy are well suited to further characterize this phenomenon.

Even though localization and transport measurements are traditional topics of condensed-matter physics, MBL is difficult to observe in real materials. This is owing to the fragility of this quantum effect to decoherence, due to coupling of the quantum many-body system to the outside world. In solid-state materials, such a coupling is often unavoidable, and caused by phonons, which interact with the electronic degrees of freedom. It turns out that AMO systems, primarily neutral atoms and ions, but also impurity spins in diamonds, are ideal systems to study many-body localization experimentally, owing to the intrinsic absence of phonons, and these systems' excellent isolation from the environment. Also, thanks to the exquisite control and observability in these synthetic quantum systems, experiments at high energy density and far from equilibrium can be realized by starting with a sudden quench of the Hamiltonian parameters. Most of the experiments performed so far, including the first clear observation of MBL in 2015, were realized in 1D systems, and probed localization by the emergence of a nonthermal steady state of the atomic density distribution or of the magnetization profile. However, later experiments using the newly developed quantum gas microscope platform, with access to individual components of the many-body system, extracted quantum entropies, or explored localization in two dimensions, in a regime where no existing theoretical method is able to predict the system behavior. The latter experiments are a prototypical example where AMO quantum simulators provide truly new insight into a difficult quantum many-body problem, and thus offer a practical quantum advantage over classical simulations.

The study of non-equilibrium quantum phenomena like MBL defines an interesting challenge to both theory and experiment. It provides a setting where new theoretical methods are required to predict even the qualitative behavior of quantum many-body systems, especially close to the transition between the ergodic (i.e., self-thermalized) and MBL phases, as well as in higher dimensions, and where experimental results are available to test such new approaches. Experimentally, even better isolation of the quantum systems from the environment is needed to reach a clearer separation of short- and long-time dynamics, and to unambiguously identify MBL in certain regimes. At the same time, the system sizes need to be scaled up to enable experimental finite-size scaling tests as a way to certify the results in regimes where no theory prediction is available. With the availability of larger systems and longer evolution times, experiments may also allow one to answer open questions about the stability of MBL to ergodic regions in higher dimensions and in the presence of interfaces, both prominent topics of current scientific debate. At the same time, better control and faster data rates are desired, for example, to scale up techniques to measure the entanglement entropy or related quantities in theoretically inaccessible regimes.

In this view, AMO experiments provide the most advanced analog quantum simulators; and one important future challenge of experiment and theory alike is to quantify the quantum advantage of these simulators. On the topic of many-body localization and far from equilibrium dynamics in general, these synthetic many-body systems provide the only available, or the most advanced, experimental platform to explore the dynamic behavior of quantum matter.

### Open System Quantum Simulation: Photonic Crystal Waveguides

The quantum simulation the committee has discussed so far refers to engineering many-body Hamiltonians and dynamics of isolated systems with ultracold atoms and molecules. In experiments, isolated systems are inevitably coupled to an environment causing decoherence, dissipation, and heating. On the other hand, physical realizations of many-body systems in quantum optical setups, where atoms are coupled to laser fields in cavities and photonic nanostructures, are intrinsically (but controllably) open systems. Here the coupling to the environment provides input and output channels: input channels provide a way of driving the system of interest with light, while output channels allow one to monitor the system by observing the emitted light in photon or homodyne detection. In a broader context, one can engineer the coupling of the many-body system of interest to quantum reservoirs, as a novel tool to generate new non-equilibrium quantum phases and as a way of obtaining entangled quantum states of interest in driven-dissipative dynamics.

An outstanding example is provided by coupling atoms or atom-like solid-state systems to photonic crystal waveguides. This area has been progressing rapidly in the past few years, and it is simultaneously at the heart of AMO science, while also touching on other disciplines, including quantum measurement theory, quantum control, materials physics, and of course quantum optics. The concept, as stressed in a recent review article, is to engineer periodic materials with a band structure that can dramatically enhance the interaction of photons with a single atom or with multiple atoms. This modified photon-atom interaction can also affect the atom-atom interaction mediated by photon modes. The modification extends control to other aspects, such as the radiative lifetime of an excited atom in such a wave-

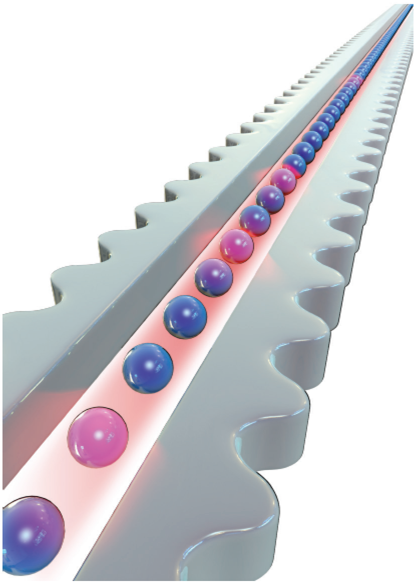

**FIGURE 3.10** A chain of atoms trapped in the guided mode of a photonic crystal waveguide. SOURCE: Reprinted figure with permission from D.E. Chang, J.S. Douglas, A. González-Tudela, C.-L. Hung, and H.J. Kimble, Colloquium: Quantum matter built from nanoscopic lattices of atoms and photons, *Reviews of Modern Physics* 90:031002, 2018, https://doi.org/10.1103/RevModPhys.90.031002, copyright 2019 by the American Physical Society.

guide. Figure 3.10 depicts such a waveguide with modifications of the light-atom interactions. The key challenge in this field involves strong coupling of coherent quantum emitters to nanophotonic systems. Recently, major advances have been made in coupling coherent atom-like emitters in diamond to nanophotonic cavities and waveguides. In particular, Silicon-vacancy (SiV) color centers have been coupled to nanoscale diamond waveguides with cooperativities approaching 100 (meaning that the color center almost exclusively exchanges energy with the waveguide optical modes and not with other modes); see also Chapter 4. Such systems have been used to realize strong optically mediated interactions between two color centers, which is a key building block of the system illustrated in Figure 3.10. Such systems are emerging as leading candidates for realization of quantum networks, discussed in Chapter 4.

### From Analog Quantum Simulation to Quantum Information Science

Analog quantum simulators, as mappings of quantum many-body Hamiltonians of interest to the “natural” Hamiltonians provided by a particular AMO platform, are, of course, not restricted to atoms and molecules in optical lattices representing Hubbard models. Other examples are spin models implemented with trapped ions or Rydberg tweezer arrays. The committee discusses these systems as programmable analog quantum simulators in Chapter 4. There exists an increasing number of control elements, such as single-site control and addressing, being added to many-body lattice systems, while keeping as a unique feature the potential scalability to a large number of particles. This positions programmable analog quantum simulators as quantum devices between the traditional quantum simulator, which is scalable to large particle numbers but with limited control, and the universal, fully programmable (digital) quantum computer. Illustrations and applications of these systems will be given in Chapter 4.

## SUMMARY OF OPPORTUNITIES AND RECOMMENDATIONS

The committee has only scratched the surface with this overview of emerging phenomena in many-body systems that can be built "from the ground up," expanding the exquisite control of single atoms (and photons) to small groups of particles and then further toward larger scales. All of the developments discussed in this chapter point toward rich opportunities for future investigations. In the few-body limit, it is of continuing interest to identify the scope of universality in quantum states, for their own intellectual interest, for their connections with many-body physics, and for the potential to add new types of controllability at both the few-body and many-body level. Ultracold molecules are starting to form a more diversified research platform, where molecular quantum gases promise to tackle a rich set of many-body phenomena, chemically interesting cold molecules will provide new insights to fundamental reaction processes, and molecules chosen for specific precision measurement targets are being brought under increasingly sophisticated levels of quantum control. Trapped ion systems, and sympathetically cooled ion-plus-atom hybrid systems, are of continuing interest, for quantum computing and simulation, and for physical chemical dynamical processes. AMO science continues to develop and extend our understanding of deeper questions such as thermalization and many-body localization, with new insights already emerging. Recent observation of a chemical reaction event within a single laser tweezer, in addition to explorations of multiple other correlated or entangled phenomena such as multiparticle tunneling between potential wells, suggest that this field is still in its early stages, and promises to grow rapidly in the coming decade.

Much of the progress in emerging quantum many-body physics with AMO has relied on extending the techniques of trapping and cooling to atoms and molecules with an increasingly complex internal-level structure, thus providing opportunities for the design of increasingly complex quantum many-body systems and exploration of novel many-body phenomena. It will be key to continue developments to extend these techniques to an increasing number of atomic and molecular species.

A unique feature of atomic and molecular quantum many-body systems is our ability to microscopically understand and characterize the properties and interactions of atoms and molecules—that is, the many-body Hamiltonians of AMO systems are in principle derivable from a microscopic theory. This is in contrast to the (often) phenomenological modeling in solid-state physics as a starting point to describe many-body dynamics. Thus, developing the theoretical tools to quantitatively predict the behavior of increasingly complex atoms and molecules is a key element for further development and leadership of AMO in designing quantum many-body systems, and achieving ultimate quantum control.

AMO quantum simulators provide us with a novel tool to study in a controlled setting equilibrium and non-equilibrium quantum many-body physics, including regimes not accessible to classical computations. This provides us first with new opportunities for discoveries in many-body physics. On the other hand, quantum simulators allow us also to generate entangled states with immediate application in quantum sensing. These connections between quantum simulation and entanglement-enhanced precision measurement are again unique to AMO physics.

While AMO provides both bosonic and fermionic Hamiltonians, such as Hubbard models, to implement analog quantum simulators, the "natural" fermions provided by fermionic atomic and molecular species are a unique feature to these simulators, where fermions are implemented on the "quantum hardware level." This is an important resource distinguishing it from both classical and quantum hardware for which complex algorithms and complex quantum gates are required in a universal digital (quantum) computer to effectively reproduce Fermi statistics. Thus, there are unique opportunities to address the problems of fermionic quantum many-body systems for both higher dimensional systems and in quantum chemistry. The 2D Fermi-Hubbard model with repulsive interactions is one of the paradigmatic examples where quantum simulators can demonstrate a regime of genuine quantum advantage. The recent breakthrough of the quantum gas microscope, possibly combined with machine learning algorithms, provides a unique AMO tool for analyzing and discovering highly correlated equilibrium quantum phases such as high-Tc superconductivity, or exploring entanglement in non-equilibrium systems. This work is closely related to the efforts in quantum information science, discussed in the following chapter. Last, the "natural" fermions provided by fermionic species in atomic quantum simulation also offer unique opportunities, as discussed in Chapter 4 in context of variational quantum simulation with Fermi-Hubbard models as the basis of programmable quantum simulators.

> **Finding:** Few-body physics continues to be of continuing interest to identify and test the scope of quantum universality, for its intrinsic intellectual interest, its connections with many-body physics, and to strengthen the controllability of both few-body and many-body quantum systems. Developing theoretical tools able to quantitatively predict the behavior and interactions of increas-

ingly complex atoms and molecules is crucial for further developments in these areas.

**Finding:** Due to recent theoretical and experimental breakthroughs, ultracold molecules now constitute a very promising research platform able to tackle diverse many-body phenomena and explorations of fundamental reactive processes, with certain molecules yielding viable targets for precision measurement science.

**Finding:** Trapped ion systems, neutral atoms, systems with long-range interactions (such as those based on molecules and Rydberg atoms) and ion-neutral hybrid systems are leading candidates for quantum information processing and simulation, and for studying chemical dynamical processes.

**Recommendation: The atomic, molecular, and optical science community should aggressively pursue, and federal agencies should support, the development of enhanced control of cold atoms and molecules, which is the foundational work for future advances in quantum information processing, precision measurement, and many-body physics.**

**Finding:** Quantum gases of atoms and molecules enable controlled exploration of equilibrium and non-equilibrium many-body physics and the generation and manipulation of entangled states applicable to quantum information processing and quantum metrology, and further developing our understanding of deep questions such as the nature of thermalization, many-body localization, and stable quantum matter away from equilibrium.

**Recommendation: Federal funding agencies should initiate new programs to support interdisciplinary research on both highly correlated equilibrium phases and non-equilibrium many-body systems and novel applications.**

**Finding:** AMO-based quantum simulators have the ability in the short term to demonstrate genuine quantum advantage over classical computational devices, without requiring the mastery of complex quantum gates required for a universal digital quantum computer. These systems can provide unique insights into complex models from condensed-matter and high-energy physics, and lead to development and testing of useful quantum algorithms.

**Recommendation: Federal funding agencies should initiate new programs involving development, engineering, and deploying the most advanced programmable quantum simulator platforms, and make these systems accessible to the broader community of scientists and engineers.**

# 4

# Foundations of Quantum Information Science and Technology

## INTRODUCTION

Quantum information science and engineering is a rapidly developing interdisciplinary field of science and technology, drawing from various subfields of physical science, computer science, mathematics, and engineering, which addresses how the fundamental laws of quantum physics can be exploited to achieve dramatic improvements in how information is acquired, transmitted, and processed. Its importance has been emphasized recently by the U.S. government through the National Quantum Initiative Act. This chapter focuses on the question of how the exquisite control of individual atoms and photons described in Chapter 3 can be brought to bear on quantum technologies for information processing. In the language of Chapter 3, a quantum information processor is essentially a quantum many-body system, far from equilibrium, whose initial state and subsequent time evolution dynamics we can control with extreme precision, and whose final quantum state can be measured ("readout") with high fidelity. Different time evolution under external control of the quantum system corresponds to running different programs (executing quantum algorithms) on the computer. The final step of measurement provides the answer to the calculation.

Theoretical research carried out over the past two decades indicates that large-scale quantum computers may be capable of solving some otherwise intractable problems with far-reaching applications in, for example, cryptology, chemistry, materials science, and fundamental physical science. These developments have stimulated a worldwide effort to build quantum machines using a variety of physical platforms, such as trapped ions, neutral atoms, superconducting circuits, spins of electrons and nuclei, and photons. The key challenges in the quest to implement scalable quantum information processors are associated with the contradicting requirements of combining excellent isolation from the environment with the ability to control strong, coherent, and programmable interactions and single-shot readout of the many-body system. The fundamental ideas of fault tolerance, established over the past two decades, suggest that it should be possible in principle to realize large-scale quantum machines despite imperfections in the individual components. Building a large-scale fault-tolerant universal quantum computer is the grand challenge of the field. However, it is currently unclear if and how this goal can be achieved within any realistic physics setting. The 2019 National Academies of Sciences, Engineering, and Medicine report *Quantum Computing: Progress and Prospects*[1] discusses the current state of the art and the challenges that lie ahead.

The power of quantum computers resides in the subtle interplay between the unique resources of superpositions and entanglement (discussed further below), in ways that are not yet fully understood. Information is physical, and binary information (bits representing zeros and ones) is stored in the two (on/off) states of transistors in ordinary computer chips. In a quantum computer, information is stored in quantum bits (qubits). A qubit is any quantum system with two discrete states. A simple example would be an atom either in its lowest energy state (ground state) or a particular excited state. Another example would be a state containing either 0 or 1 photons of some particular energy. Qubits can be in superposition states in which we are uncertain whether they will yield 0 or 1 when measured (and indeed the measurement results are ineluctably random—a feature that can be used to make true random number generators). At first glance, this appears to be a major bug, not a feature. However, it is now understood that (very crudely speaking) qubits have the potential to be 0 and 1 simultaneously, creating a kind of quantum parallelism that is one of the sources of power of the quantum computer. The other distinctly quantum resource is entanglement, which will be described further below.

Even though recent experimental advances already allow for unprecedented new insight into the physics of complex quantum many-body systems, it is currently unclear if large-scale quantum processors can be used to obtain substantial speed-up over classical computers for any practical tasks apart from simulating complex quantum systems and Shor’s factoring algorithm. This is a key challenge that theoretical quantum computer science must address in the coming decade. It seems virtually certain that the small-scale quantum computers that are beginning to become available will allow numerous people from a variety of disciplines to start playing with them and coming up with new and unexpected ideas for how best to

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[1] National Academies of Sciences, Engineering, and Medicine, 2019, *Quantum Computing: Progress and Prospects*, The National Academies Press, Washington, DC.

operate them and improve their performance, just as occurred in the early history of classical computation. Frustration with the extreme difficulty of programming early classical computers using electrical plug boards and patch cords led directly to the invention of the von Neumann architecture in which data and instructions are stored in memory in the same way, so that programs could modify their own instructions. If we are fortunate, the next decade will lead to analogous breakthroughs in the quantum computation domain.

In this chapter, the committee discusses key ideas and hardware-level techniques for understanding fundamental principles behind creating, quantifying, and controlling quantum entanglement and universal control of many-body quantum systems, as well as for development of technological platforms for quantum information processing and simulation, quantum communication networks, and the application of quantum information ideas for enhanced sensing and measurement.

Ideas, techniques, and methods of atomic, molecular, and optical (AMO) physics are at the forefront of this exciting frontier involving building, studying, and applying large-scale controlled quantum systems. Experimental efforts to manipulate large-scale quantum systems are achieving steadily improving results. AMO systems and techniques played a pioneering role and continue to play a leading role in this field. Programmable quantum systems of up to about 50 quantum bits have been realized using trapped ions, neutral atoms, and superconducting circuits. Ion trap quantum computers represent the gold standard of qubit coherence and quantum control, and were recently used to realize sophisticated algorithms for quantum chemistry. Recent developments involving realization of programmable neutral atom arrays in various spatial dimensions, and quantum operations using controlled excitations into atomic Rydberg states, demonstrate the promise for high-fidelity control of systems composed of hundreds of qubits. Furthermore, atom-photon interfaces are being developed, which convert “stationary qubits”—for example, stored in atoms as quantum memory—to “flying qubits” represented by microwave or optical photons propagating—for example, in waveguides—as building blocks for both local and wide-area quantum networks. This implementation of coherent quantum operations in quantum networks provides a basis for fault-tolerant quantum communication including quantum repeaters (QRs), and the potential for scaling up quantum computers in modular architectures. The extensions of the methods originally developed in the AMO community to solid-state systems, such as circuit quantum electrodynamics (QED), play a central role in the most advanced superconducting quantum computer realizations. In particular, they form the basis for recently demonstrated promising approaches for quantum error correction.

At the same time, the fundamental concepts of quantum entanglement and quantum coherence now play central roles in almost all subfields of physical science. Aside from setting the stage for quantum technologies, research on quantum entanglement, quantum information processing, and quantum error correction is also establishing new tools and approaches for deepening our understanding of fundamental physical phenomena. For example, in quantum condensed-matter physics, concepts arising from the study of quantum entanglement have spurred the development of powerful methods for classifying quantum phases of matter and more efficient schemes for simulating entangled quantum many-body systems using conventional classical computers. In addition, ideas from quantum information theory and quantum entanglement theory may deepen our understanding of the quantum structure of spacetime.

In the next decade, these experimental and theoretical methods will allow researchers to start implementing and testing novel quantum algorithms for diverse scientific applications, and to explore practical methods for quantum error correction and fault tolerance. They could enable the first realizations and tests of quantum networks with applications to long-distance quantum communication and nonlocal quantum sensing. In addition, controlled quantum systems are already being exploited in some of the world's most precise atomic clocks, and in magnetic sensors that achieve an unprecedented combination of sensitivity and spatial resolution. Meanwhile, as already mentioned in Chapter 3, new experimental tools are being harnessed to simulate models of quantum many-body physics that are beyond the reach of today's digital computers.

Exciting new scientific opportunities are arising at the interface of AMO physics, quantum information science, device engineering, condensed-matter physics, and high-energy physics: this new scientific interface is by now often referred to as quantum information science and engineering. For example, advances in precision measurements exploiting quantum coherence and entanglement may enable unprecedented tests of fundamental symmetries of the universe as well as new strategies for probing dark matter and dark energy (see also Chapter 6). Quantum simulators and quantum computers may provide new insights regarding the behavior of strongly correlated many-body systems and strongly coupled quantum field theories relevant to high-energy particle physics as well as condensed matter. Furthermore, concepts from particle physics and quantum field theory may suggest new applications for quantum computers, and new ways to make quantum systems more robust against noise. From this perspective, this chapter plays an important role connecting basic tools of quantum control for photons and atoms presented in Chapters 2 and 3 to some emerging applications presented in Chapters 5, 6, and 7.

## UNDERSTANDING, PROBING, AND USING ENTANGLEMENT

Entanglement is the most precious property and resource of quantum physics, and fundamentally distinguishes quantum physics from classical physics. It occurs when two or more objects possess certain correlations, which cannot be explained classically in terms of local hidden variables or quantum-mechanically in terms of product states or mixtures thereof. In the context of quantum technologies, entanglement is a resource in the sense that the more entanglement, the better one can perform particular tasks such as quantum communication or computation. This is why the study and quantification of entanglement plays a central role in quantum information theory, the discipline that develops the theory behind applications of quantum physics to the transmission and processing of information.

Entanglement of simple systems, composed of only a few objects, is by now relatively well understood. For pure states (i.e., states of systems not entangled with external environmental degrees of freedom inaccessible to the experimenter), the presence or absence of entanglement can be easily certified. Regarding the quantification, the situation is more complex. For two systems, the entanglement is properly quantified by the entropy of entanglement, $E$, which measures how mixed the local (reduced) states are in terms of the von Neumann entropy. The maximally entangled states of two qubits (so-called Bell states) possess one unit of entanglement; the entanglement of other states is related to that unit in the sense that they can be converted to Bell states at a ratio given by $E$. For multipartite states, the situation is more complicated, as one can define different measures, and there is not even a partial order with respect to any of them—that is, one state can be more entangled than another according to one measure, but less according to a different measure. In that case one typically considers the pragmatic approach of operational measures, which are task dependent, meaning that they are defined according to the advantage they yield for a given informational task. For mixed states, the situation is even more intricate. While it is possible to determine whether states are entangled or not, in some cases it may become a difficult computational task. The quantification faces the same problems as for pure states. Despite a lot of progress made over the past decade, the theory of entanglement is still not fully established.

The past 10 years have experienced substantial progress in probing entanglement in experiments. First, different strategies have been proposed to detect the presence of that intriguing property in few- or even many-body systems. These strategies have been widely used in a variety of experiments in order to benchmark their performance, or to certify their quantumness. Experiments with tens of trapped ions, atoms, superconducting qubits, and other systems have witnessed the presence of the strongest forms of entanglement, while other experiments with many particles (for instance, atomic ensembles with millions of atoms) have also detected some weak forms of entanglement. Each of these can be considered as a "tour de force" in experimental physics, and have successfully demonstrated that close theory-experiment connection can lead to rapid progress.

Apart from the development of a deeper understanding of entanglement as well as its quantification as a resource, there remain important challenges for future research. On the experimental side, there is the demonstration of higher levels of entanglement with different technologies, as well as the possibility to entangle more objects together strongly (for example, in so-called Greenberger–Horne–Zeilinger [GHZ] states). An experimental challenge would be to create such a state of *N* qubits, or N00N states of photons, which are useful in the context of parameter estimation, metrology, and sensing. (So-called N00N states are maximally entangled states consisting of a coherent superposition of two possibilities: *N* photons in mode 1 and 0 photons in mode 2, superposed with 0 photons in mode 1 and *N* photons in mode 2. The origin of the name can be seen in the standard quantum notation for such a state: |N0>+|0N>.) From the theory side, finding new applications of entanglement would be highly desirable. Nowadays, we know of only a few tasks for which quantum properties (and, in particular, entanglement) can improve performance. Among these are cryptography, random number generation, quantum computing, and sensing. However, there may be many other realms where entanglement provides an advantage over classical limits. The further development of the theory of entanglement may well lead to such applications in the next decade.

In the past few years, we have witnessed how the notion of entanglement has gone beyond quantum information theory and had a strong impact in other areas of physics. For instance, it has been found that in the quantum ground state, and as long as interactions are local, entanglement is relatively scarce in nature as it typically fulfills a so-called area law. In brief, this means that the entanglement (or, more precisely, the quantum mutual information) of a region with respect to its complement scales with the surface area of the region and not with the volume. This occurs in many domains of physics, including atomic, condensed-matter, and high-energy, and has striking consequences. This implies that the corresponding states can be efficiently described in terms of tensor networks, a new language that allows one to overcome the exponential growth of information that is normally required to describe and deal with such systems and that prevents the analysis of quantum many-body systems in general. Thus, a great challenge of entanglement theory is to help to develop algorithms that allow one to address physics questions that cannot be attacked with classical (super) computers. Furthermore, the study of entanglement has expanded to other areas of physics including quantum gravity, where several theories have recently emerged that connect entanglement with other concepts. In particular, entanglement is at the core of the so-called firewall paradox (of black holes), and it has been used to devise toy-models (of condensed-matter many-body theories) and to understand some aspects of holographic principles (in theories of gravity), and is possibly even connected to the emergence of the geometry of space-time itself. In particular, entanglement has established a common language in all those communities, and it is expected to shed new light in different areas of physics.

It is important to emphasize that recent advances in realizing quantum machines allow one to study the fundamental aspects of quantum entanglement in the laboratory. In particular, the experimental systems described in this chapter allow researchers to experimentally probe various aspects of quantum many-body systems using trapped ions and neutral atoms. In addition, the completion of several "loophole free" experimental tests of Bell inequalities,[2] described below in the section "Bell Inequalities, Quantum Communication, and Quantum Networks," was one of the highlights of the past decade. These sophisticated tests were made possible by remarkable experimental advances, which in turn play a crucial role in quantum technologies. Furthermore, Bell tests are also used in the very core of some quantum technologies, such as Device Independent Quantum Key Distribution (DIQKD), and ultimate quantum random number generators (QRNGs).

## CONTROLLING QUANTUM MANY-BODY SYSTEMS

AMO systems provide one of the most advanced and promising ways to implement controlled quantum systems. Ideas, techniques, and methods developed in the framework of AMO define the forefront of building, studying, and applying large-scale quantum information processing, and also have a profound impact in helping develop a similar level of control in solid-state systems. Individual atoms, first of all, host the most pristine qubits found in nature. Atoms, by their very nature, are identical, and when isolated from detrimental effects of the environment using well-developed atomic techniques of trapping and cooling, provide us with large-scale quantum registers of identical qubits. When atomic qubits are represented by appropriate internal energy levels within individual atoms, they are essentially atomic clocks and hence enjoy the attributes of high-performance frequency standards. Second, the long tradition in AMO of precision measurement has provided the community with the tools, including lasers and microwave fields, which provide the necessary control techniques to manipulate atoms and their interaction, as well as high-fidelity readout, fulfilling the stringent requirements of control of engineered large-scale quantum matter. In an effort to scale quantum devices to an increasing number of quantum particles, atomic physics has the unique advantage that sophisticated quantum error correction techniques might not be as much the limiting requirement as in other physical settings—even though the development of these techniques is one of the key challenges in the field. Last, atomic systems provide natural quantum interfaces, or transducers, where "stationary qubits" stored in atomic quantum memory are interfaced with, for example, optical or microwave photons as "flying qubits," as required in building "on chip," intra-laboratory, or wide-area quantum networks.

Below, recent highlights are presented demonstrating the progress, future promise, and challenges associated with quantum control of large-scale, many-body atomic systems. Ion trap quantum systems have long represented the gold standard

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[2] A. Aspect, Viewpoint: Closing the door on Einstein and Bohr's quantum debate, *Physics* 8:123, 2015, 10.1103/Physics.8.123.

of qubit coherence and quantum control. Recently, they were used to realize sophisticated quantum algorithms. New developments involving realization of configurable neutral atom arrays in various spatial dimensions, and quantum operations using controlled excitations into atomic Rydberg states, demonstrate the promise for high-fidelity control of systems composed of hundreds of qubits. At the same time, the extension of the methods originally developed in the AMO community to solid-state systems, such as circuit QED, play a central role in the most advanced solid-state quantum computer realizations. Last, AMO methods and techniques are employed for controlling electronic and spin degrees of freedom of atom-like impurities in solid-state systems, with applications ranging from implementation of quantum networks to nanoscale quantum sensing.

## Trapped Ion Quantum Computing

For the past two decades, trapped atomic ions have been among the most advanced candidates for the implementation of quantum processors (see Figure 4.1). Following very early proposals and demonstrations of controllable quantum entanglement operations in the mid-1990s, there are now more than 50 teams investigating trapped ion entanglement and quantum computing architectures in academic institutions, national laboratories, and industrial organizations around the world. In addition to the continued refinement of fundamental entanglement operations and protocols with trapped ions, this platform is becoming systematized and controlled by agile hardware interfaces and software technology in a way that is moving toward practical quantum computation. This is catalyzed by the fact

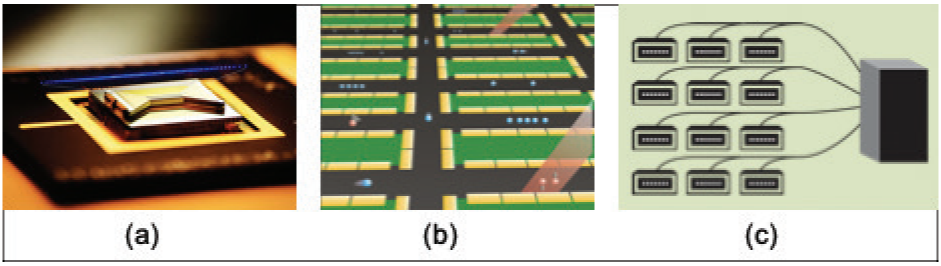

**FIGURE 4.1** Trapped ion qubits and scaling of trapped ion quantum computer systems. (a) Photograph of a semiconductor chip trap with gold-plated electrodes (bowtie shape) is composed of many electrodes that suspend an array of individual atomic ions above the surface of the chip. Eighty $^{171}Yb^+$ ions are confined in a linear array, with an end-to-end distance of about 0.3 mm and floating 0.08 mm above the chip surface (trap fabricated by Sandia National Laboratories). (b) Schematic: scaling of trapped ion systems by shuttling qubits between multiplexed zones on a complex ion trap structure. (c) Modular scaling to very large numbers of qubits using photonic interconnects between elements of an array of individual trapped ion crystals. SOURCE: (a) and (c): C. Monroe, private communication. (b) D. Leibfried, private communication.

that the scaling of trapped ion quantum computers does not rely on new physics or even breakthroughs, but on the engineering, systemization, and improved performance of their controllers. Importantly, it appears likely that trapped ion quantum computers will be able to scale to dimensions well beyond those needed for quantum advantage in practical problems, that is, demonstrating tasks beyond what can be achieved efficiently on classical devices.

As noted above, individual trapped and laser-cooled atoms and ions host the most pristine qubits found in nature, and the highest performing individual atomic clock systems are based on atomic ions. By virtue of their electrical charge, individual atomic ions can be isolated and manipulated in space with exquisite precision. By applying external electromagnetic fields from nearby arrays of electrodes inside a vacuum chamber, individual atomic ions can be confined or trapped for indefinite periods of time The most popular atomic ion species used for quantum computing purposes are those with single valence electronic configurations such as $Be^+$, $Ca^+$, and $Yb^+$, whose essential attributes are the required laser wavelengths for cooling and manipulation, the electronic structure of the atom—primarily its nuclear spin and ancillary electronic energy levels—and the atomic mass.

When laser-cooled, a collection of trapped atomic ion qubits forms a crystal, and established techniques using lasers and microwaves allow the initialization and measurement of quantum states within trapped ion qubits with nearly perfect fidelity. Moreover, following classic nuclear magnetic resonance (NMR) and atomic clock techniques using microwaves or optical fields, individual qubit operations such as single-qubit gates or rotations, can be achieved with greater than 99.99 percent fidelity.

The Coulomb interaction between atomic ions in a crystal leads to strongly coupled normal modes of motion, much like an array of pendula connected by springs. These modes can be utilized as information buses to generate programmable entanglement between the qubits. The generation of entangled quantum logic gates between trapped ion qubits relies on qubit state-dependent forces (from applied optical or microwave fields). The fidelity of two-qubit gates has reached the 99.9 percent level using both optical and microwave fields, and is currently limited by mechanisms such as spontaneous emission or motional decoherence during the gate, residual intensity fluctuations of the control beams, stability of the frequency of the motional modes, and the decoherence of the qubit itself. It is important to realize that the error budgets in these systems are well characterized, and research efforts continue to improve gate performance in these systems.

Based on the high-fidelity component operations demonstrated to date, small-scale ion trap systems have been assembled in which a universal set of quantum logic operations can be implemented on small qubit systems in a programmable manner, forming the basis of a general-purpose quantum computer. While the performance of individual quantum logic operations in these fully functional systems tends to lag behind the state-of-the-art demonstrations at the component level of just two qubits, the larger systems can exhibit a wide variety of quantum algorithms and tasks that comprise some of the largest and most complex quantum computer systems operated to date. For instance, small-scale trapped ion systems have been used to implement Grover's search algorithm, Shor's factoring algorithm, the Deutsch-Jozsa algorithm, quantum Fourier transform, the Bernstein-Vazirani algorithm, the quantum hidden shift algorithm, quantum error correction and detection codes, and quantum simulation tasks.

While it appears possible to scale a trapped ion quantum computer to 30-100 qubits in a single crystal, it may prove difficult to push well beyond this level given technical limitations such as trap potential fluctuations and other slowly varying control parameters. However, there are many opportunities to scale trapped atomic ions using more modular approaches. At the lowest level, a very large chain can be rigidly displaced through an interaction/control zone much like a tape moves across a head in a classical Turing machine. The physical shuttling of atomic ions through separated trapping zones in sufficiently complex trap electrode geometries is a promising method for a modular quantum computer architecture, sometimes called a "quantum CCD," as shown in Figure 4.1(b). This may require multiple species of trapped ions for sympathetic cooling after splitting/merging chains, and also cryogenic (4 K) environments to maintain low pressure and long-chain lifetime. Great progress has been achieved in the ability to integrate quantum gate operations with shuttling between collections of trapped ion qubits. This has been demonstrated so far on the level of a few ions, and one of the future challenges is scaling to many thousands of qubits on a single chip using this method.

A higher level of modularity may be afforded by exploiting the interface between trapped ion qubit memories and flying photonic qubits, as depicted in Figure 4.1(c). Here, certain "communication" qubits in a chain are linked to other such qubits in a spatially separated chain, perhaps on another ion trap chip, or in a separate vacuum chamber over longer distances. This architecture follows closely the multicore architecture adopted by classical computing processors, and follows from the generalization that complexity demands modularity.

In general, the scaling of qubits toward a useful large-scale quantum computer requires that both qubits and gate quality do not degrade with increasing size of the system. Given pairwise gate operations between qubits, it might be expected that with N qubits, we will require $N^2$ coherent gate operations. This would call for either error correction before N gets too large or for gate fidelities to be improved as $1-1/N^2$. Not only is this a scaling benchmark that allows full entanglement within a system, but also many applications demand this form of scaling. This evolution of the technology is particularly challenging, as larger quantum systems generally couple more strongly to their environment. At present, trapped ions are among the leading platforms for quantum information processing having achieved full quantum control for 20 and more qubits. In the foreseeable future, atomic ion qubits will be limited mainly by their controllers. In addition, the error modes of trapped ion devices are well understood, offering great confidence that trapped ion quantum computers will indeed scale to dimensions far beyond what is achieved in present experiments.

### From Quantum Computers to Programmable Quantum Simulators

Programmable quantum simulators (PQSs) have recently emerged as a new paradigm in quantum information processing. In contrast to the universal quantum computer, PQSs are nonuniversal quantum devices with restricted sets of quantum operations, which however can be naturally scaled to a large number of qubits. PQSs are experimental platforms that are able to produce families of interesting quantum states by letting large collections of particles interact in a precise fashion, thus generating potentially large-scale entanglement. The resulting quantum many-body states can be further manipulated via precise single-particle control. The quantum states produced in this way are thus programmable in the sense that they are parametrized by control parameters provided by the experimentalist (such as duration and strength of the interaction, and degree of single-particle rotations). In contrast to universal quantum computing, generation of these quantum states is not universal—that is, they belong to a restricted class of states, yet they are the ones for which interesting applications exist (to be discussed below). PQS platforms can be viewed as an interpolating step between dedicated, single-purpose quantum simulators and fully fledged universal quantum computers. As more and more refined control is developed, PQS platforms can be expected to bridge and ultimately close the gap between these two notions.

Significant progress has been made in the development of PQSs. The specialization of these platforms to a single task endows them with relatively good scaling properties compared to universal quantum computing devices such as quantum computers, not only regarding the number of particles or qubits, but also in the fidelity of quantum operations they can perform. Furthermore, imaging methods such as quantum gas microscopes for optical lattices or the spin readout of trapped ions and atomic arrays provide detailed access to the properties of the quantum states at single-particle resolution. Repetition rates of the experimental cycles have increased tremendously, enabling large numbers of experiments to be performed in short times. Particular examples of PQS platforms are, for instance, linear arrays of trapped ions, as discussed in the previous section (see Figure 4.1), and arrays of trapped atoms in optical tweezers that can be excited to the Rydberg state (see below, and Figures 4.3, 4.5, and 4.6a,b). Both platforms realize controllable Ising-type interactions that can be switched on and off at will.

All of these recent advances have opened the door to novel applications, beyond traditional analog quantum simulation for which the platforms were originally intended. A key example is the use of the PQS as a quantum co-processor in a hybrid classical-quantum feedback loop. The PQS is employed in its role as a quantum state generator, controlled by a classical computer that attempts to steer the resulting quantum state toward a desired target state. The targeted state can be the ground state of a physical model (see Box 4.1). An alternative application would be to encode an optimization problem in the many-particle state and let the quantum

## BOX 4.1
## Variational Quantum Simulation

A seminal application of PQS has been found in the context of variational quantum simulation, in which a classical computer is interfaced with a quantum co-processor in a closed feedback loop. Variational quantum simulation (VQS) can be understood as an optimization procedure in which the quantum system takes care of the classically difficult task of evaluating the cost function to be optimized, by sampling from highly entangled quantum states created by the quantum co-processor. Once the optimal control parameters have been found, the quantum state can be prepared at will and is available for further study. Depending on the cost function to be optimized, VQS opens the door for diverse applications, ranging from the preparation of nontrivial many-body states to highly entangled quantum states useful for quantum metrology applications (see Figure 4.1.1).

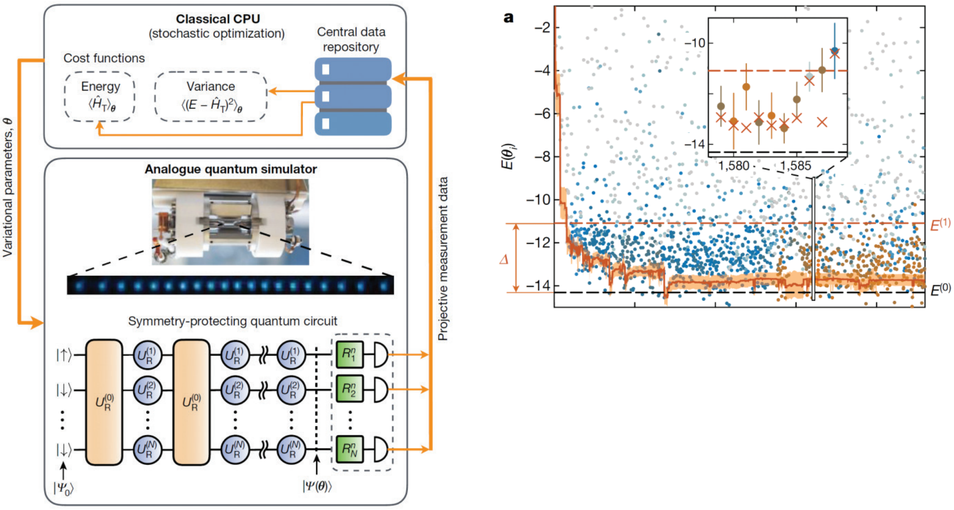

**FIGURE 4.1.1** *Left:* Sketch of the quantum-classical feedback loop, where quantum states are generated by a parameter (denoted by θ)-dependent quantum circuit consisting of entangling interactions (yellow boxes) followed by single-particle rotations (blue circles). Projective measurements are then reported back to the classical computer, which evaluates a cost function that is optimized over the parameter vector θ. *Right:* Optimization trajectory (energy versus iteration number) obtained on a programmable 20-qubit ion trap quantum simulator, when optimizing the energy of a quantum many-body system. SOURCE: Reprinted by permission from Springer Nature: C. Kokail, C. Maier, R. van Bijnen, T. Brydges, M.K. Joshi, P. Jurcevic, C.A. Muschik, P. Silvi, R. Blatt, C.F. Roos, and P. Zoller, Self-verifying variational quantum simulation of lattice models, *Nature* 569:355-360, 2019, https://doi.org/10.1038/s41586-019-1177-4, copyright 2019.

system generate approximate solutions using the Quantum Approximate Optimization Algorithm (QAOA). In both cases, many short experiments with only modest requirements on coherence time are performed, and the resulting state is measured frequently. At each step, a cost function is evaluated from the measurements, which the classical computer attempts to optimize variationally in a feedback loop.

Future experimental efforts should continue to improve the quality of available PQS platforms by increasing the coherence times and the number of particles and extending the set of available controls. Improved repetition rates of experiments would be beneficial for the use of PQSs in variational settings. The latter point is particularly relevant for itinerant atomic systems, such as fermionic atoms in optical lattices (see Chapter 3), whose application in a variational optimization context could open interesting perspectives to address long-standing equilibrium problems in quantum chemistry, condensed-matter, and high-energy physics. Theoretical efforts should be directed at quantifying the computational power of PQS platforms in the context of solving optimization problems, and exploring how PQSs could function as modular building blocks for a future generation of quantum simulators and quantum computers. A further theoretical focus area is the development of novel applications of the quantum states produced by PQS, for instance in quantum metrology.

Controllable, coherent many-body systems can provide insights into the fundamental properties of quantum matter, can enable the realization of new quantum phases, and could ultimately lead to computational systems that outperform existing computers based on classical approaches. Recently several experimental groups in the United States and France developed and demonstrated a powerful new method for creating controlled many-body quantum matter that combines deterministically prepared, reconfigurable arrays of individually trapped cold atoms in one, two, and three spatial dimensions with strong, coherent interactions enabled by excitation to Rydberg states (see, e.g., Figure 4.2).

For example, recent experiments realized programmable quantum spin model with tunable interactions and system sizes of up to 51 qubits. This work already led to the discovery of a new class of quantum many-body states that challenge traditional understandings of thermalization in isolated quantum systems, and has triggered extensive new theoretical investigations into these so-called quantum many-body scars. Using the same platform and applying it to the study of condensed-matter models, these experiments observed quantum phase transitions into spatially ordered states that break various discrete symmetries. The experimental study of quantum critical dynamics within this platform offered the first experimental verification of the quantum Kibble-Zurek hypothesis, and showed its application to exotic, previously unexplored models such as the chiral clock model. In addition, a similar platform was recently utilized for realization of symmetry-protected topological phases of matter.

Apart from studies of many-body quantum physics, recent experiments demonstrated the suitability of the platform for quantum computation by overcoming

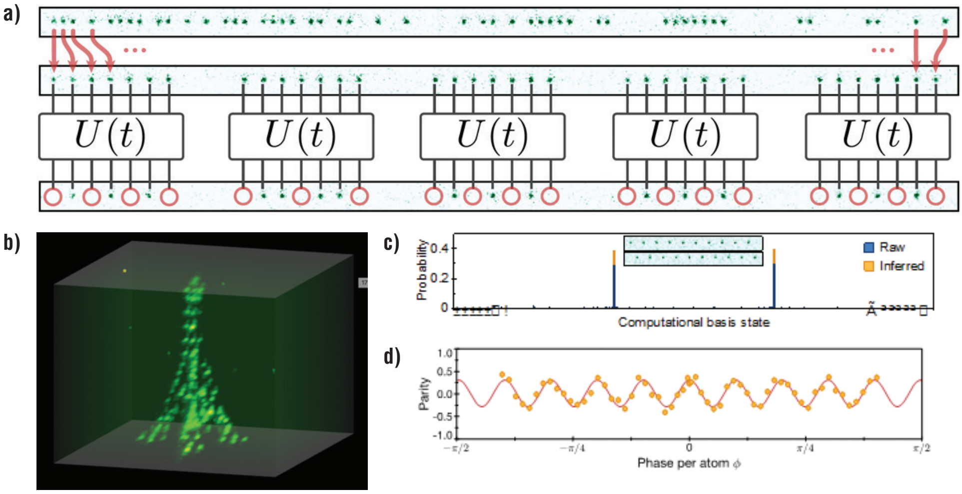

FIGURE 4.2 (a) Individual atoms in tweezer arrays can be arranged in desired spatial configurations. Programmable interactions are engineered via their controlled excitation into Rydberg states. (b) Sophisticated geometries of atoms can be prepared in both 2D and 3D, as demonstrated here by fluorescence imaging of a 3D structure of atoms. Highly entangled states, such as GHZ-type states, in which an entire array of atoms is fully correlated, can be prepared. The measurements of the 20-atom density matrix populations (c) and coherences, as evidenced by measured parity oscillations (d), indicate entanglement of a 20-atom system, the largest GHZ state prepared to date. SOURCE: (a) Endres et al., *Science*, 354, 1024 (2016). (b) Reprinted by permission from Springer Nature: D. Barredo, V. Lienhard, S. de Léséleuc, T. Lahaye, and A. Browaeys, Synthetic three-dimensional atomic structures assembled atom by atom, *Nature* 561:79, 2018, https://doi.org/10.1038/s41586-018-0450-2, copyright 2018. (c-d) From A. Omran, H. Levine, A. Keesling, G. Semeghini, T.T. Wang, S. Ebadi, H. Bernien, A.S. Zibrov, H. Pichler, S. Choi, J. Cui, M. Rossignolo, P. Rembold, S. Montangero, T. Calarco, M. Endres, M. Greiner, V. Vuletić, and M.D. Lukin, Generation and manipulation of Schrödinger cat states in Rydberg atom arrays, *Science* 365(6453):570-574, 2019, doi:10.1126/science.aax9743, reprinted with permission from AAAS.

several long-standing limitations in quantum control of cold atoms. High-fidelity single-qubit rotations and quantum state detection has been demonstrated. In addition, the preparation of high-fidelity entangled states has been demonstrated, establishing neutral atoms as a competitive platform for quantum information processing. Most recently, this system has been used by Harvard-Massachusetts Institute of Techology (MIT) collaboration to realize GHZ entangled states of 20 atoms, which is the largest *N*-particle entangled state of individually measured particles to date. At the time of the writing, high-fidelity multi-qubit operations have been realized by the groups at Harvard/MIT and Wisconsin using this approach. Last, recent theoretical work demonstrated that this approach is well suited for realization and testing of quantum algorithms for solving complex combinatorial optimization problems, paving the way toward exploring the first real-world applications of quantum computers.

Before concluding, the committee notes that this is a very rapidly growing area of research. Very recently, a number of new systems involving optical tweezer arrays have been demonstrated. These include new experiments involving realization of tweezer arrays with alkaline-earth atoms such as strontium and ytterbium, as well as polar molecules (see Chapter 3). These platforms hold promise for many potential applications, ranging from high-fidelity quantum information processing and quantum simulations to quantum metrology.

### Cavity and Circuit QED

QED is the theory of the interaction of light quanta (photons) with electrons and atoms. As described below, one of the exciting developments in the past 15 years has been the movement of ideas from AMO physics and quantum electrodynamics into the world of condensed-matter physics.

QED correctly predicts many subtle phenomena and is widely considered to be the most successful and most precisely tested theory in all of science. One of its most fundamental predictions is that atoms placed into excited states are unstable and will spontaneously fluoresce—that is, decay to a lower energy state by emitting one or more photons. This useful phenomenon is crucial for many technologies including computer screens and other types of optical displays.

Ordinarily, photon modes of all possible wavelengths (and hence energies) are available, and thus the atom can always find a mode of the correct energy into which it can decay. In cavity QED, one modifies the photon modes available to the atom by placing it between two highly reflecting mirrors to form a resonant cavity that can support only modes of certain discrete wavelengths. Cavity QED allows one to engineer the photon environment seen by the atom and thereby either enhance or suppress its decay rate. These so-called Purcell effects have been observed in optical and microwave cavities but are typically rather weak and limited by the small size of the atom and the small wavelength of light relative to the large electromagnetic mode volume of the resonator.

Inspired by ideas from condensed-matter physics and electrical engineering radio filter theory, AMO scientists have in recent decades made great progress in creating optical resonators with very small mode volume—comparable to the volume associated with a single wavelength of the light emitted by the atom. One way to accomplish this is by custom design of so-called photonic bandgap materials. These structures can be engineered to efficiently couple the light emitted by a single atom (or color center defect in a solid) into an optical fiber for purposes of quantum control, communication, and information processing. Since the relevant scale against which to measure cavity mode dimension is the wavelength of the photons it traps, one can effectively decrease the mode volume by moving to atoms that emit and absorb long wavelength microwave photons rather than short wavelength optical photons. Serge Haroche shared the 2012 Nobel Prize for his work on cavity QED of Rydberg atoms passing through a microwave resonator.

Rydberg atoms are ordinary atoms with one electron excited to a large orbit around the nucleus. Here "large" means about $10^4$ atomic diameters or $10^{-6}$ m. In the past 20 years, condensed-matter physicists have gone even further by constructing artificial atoms out of superconducting Josephson junction circuits. These millimeter-size objects are visible to the naked eye and contain trillions of electrons. However, because of their superconductivity, the electrons in these circuits move coherently in unison, allowing the "atoms" to have quantized energy spectra simpler even than hydrogen. Because of their enormous size, these quantum objects interact very strongly with electromagnetic waves. In free space, these "atoms" spontaneously decay very rapidly by emitting microwave photons. However, unlike the case with optical photons, one can completely enclose these "atoms" inside a superconducting box that effectively acts like a nearly perfectly reflecting set of microwave mirrors fully surrounding the "atom." This makes it almost impossible for the "atom" to spontaneously decay (because the microwave photons keep getting reflected back and cannot escape), thereby extending the lifetime of the artificial atoms through the Purcell effect by a factor of $10^3$. With this strong lifetime enhancement, artificial atoms have coherence times relative to their transition frequencies that are comparable to the hydrogen atom. The Purcell effect can also be used to shorten the lifetime by placing the atom in resonance with the cavity. A spectacular example of this is recent work using a resonant cavity to dramatically enhance the spontaneous emission rate of donor electron spins in silicon by a factor of nearly $10^{12}$, thereby shortening the spin relaxation time by a factor of $10^3$. One application of this enhanced dissipation is spin reset in magnetic resonance experiments and qubit control experiments.

The fact that a cm-scale microwave cavity can have a mode volume considerably smaller than a cubic wavelength further enhances the coupling of the artificial atom to photons trapped in the cavity. The coupling is so strong that even when the "atom" and cavity are detuned in frequency from each other by 20 percent, the second-order effects of the "atom" virtually emitting and quickly reabsorbing photons to and from the cavity yields an ultrastrong dispersive interaction $H = \chi\sigma^z a^\dagger a$, where $\sigma^z$ describes the state of the (two-level) "atom" and $\hat{n} \equiv a^\dagger a$ represents the number of photons in the cavity. The meaning of this dispersive interaction is that the transition frequency of the "atom" suffers a quantized "light shift" for each additional microwave photon present in the cavity. It also means that the cavity has two different resonance frequencies depending on whether the "atom" is in its ground or excited state. Remarkably, the dispersive coupling $\chi$ can be three orders larger than the linewidths (decay rates) of both the cavity and the "atom," placing this system in a completely new regime of nonlinear quantum optics at the single-photon level.

This ultrastrong coupling relative to dissipation permits universal control of the combined qubit-cavity system. One can readily make quantum nondemolition (QND) measurements of photon number: measure the photon number parity $\hat{P} = e^{i\pi a^\dagger a}$ (without measuring the photon number), and using these parity measurements, carry out complete state tomography through direct measurement of the Wigner function (a quasi-probability distribution in phase space). These capabilities go far beyond what is possible in ordinary quantum optics where the nonlinear interactions of light and matter are much weaker relative to the dissipation. Figure 4.3 illustrates these quantum control and measurement capabilities.

This powerful ability to control quantum states opens up a new regime of strong nonlinear quantum optics at the single-photon level. It permits creation of error-correctable logical qubits, not from material objects, but rather from superpositions of different numbers of microwave photons. These "photonic logical qubits" are the first qubits in any technology to reach the breakeven point for error correction (where the lifetime of the quantum information encoded in the logical qubit exceeds that of any individual physical qubit). Other recent advances include deterministic teleportation of quantum gates on logical qubits, and novel new entangling gates such as the exponential-SWAP gate that acts on two microwave resonators by performing a coherent superposition of swapping and not swapping the contents of the two resonators. These capabilities advance the possibility of gate-based photonic quantum computing and also of simulating the many-body dynamics of interacting bosons. An exciting new direction would be using an array

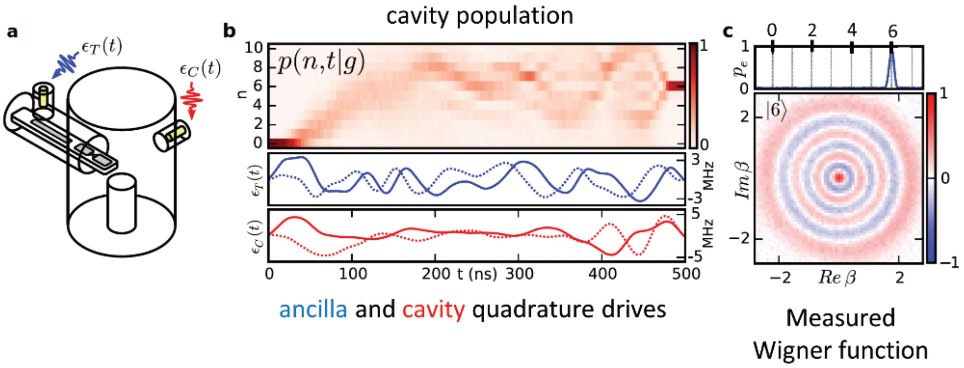

**FIGURE 4.3** Creation and verification of an n = 6 photon Fock state in a superconducting resonator using numerically optimized microwave control signals applied to the resonator and to the transmon artificial atom ancilla. (a) Superconducting microwave resonator coupled to an artificial atom. (b) Upper panel shows the probability distribution of photon numbers in the cavity during the application of microwave drives whose amplitudes versus time are shown in the lower two panels. (c) Top panel: final photon number distribution. Lower panel: The characteristic "bullseye" shape of the measured Wigner function confirms that the system ends up in the quantum state with precisely 6 photons. SOURCE: R.W. Heeres, P. Reinhold, N. Ofek, L. Frunzio, L. Jiang, M.H. Devoret, and R.J. Schoelkopf, Implementing a universal gate set on a logical qubit encoded in an oscillator, *Nature Communications* 8:94, 2017, doi:10.1038/s41467-017-00045-1, Creative Commons Open Access.

of microwave cavities to simulate the fractional quantum Hall effect for bosons in the parameter regime where the excitations are Majorana zero-modes obeying non-Abelian statistics. Another exciting new direction that is now rapidly blossoming is "quantum acoustics," in which one can use similar techniques to create, control, and measure individual quanta of sound (mechanical vibrations).

## CONTROLLED MANY-BODY SYSTEMS FOR QUANTUM SIMULATIONS

### Simulating Quantum Dynamics of Many-Body Systems

Quantum simulation of complex many-body systems was the original context in which Richard Feynman proposed building programmable quantum machines. The motivation was that exact classical computation or simulation of quantum dynamics becomes extremely challenging even for a modest-size quantum system. In fact, it is virtually impossible to exactly compute the dynamics of coupled qubits with system sizes exceeding around 50 quantum bits. These considerations make it very challenging to study non-equilibrium dynamics of closed quantum systems. Central to such systems is the dynamics of entanglement growth that creates nontrivial quantum correlations that cannot be captured by simple theories. Recent experimental advances involving programmable quantum simulators already allow researchers to carry out quantum simulations with system sizes that cannot be handled classically, and to gain unprecedented insights into the physics of such systems.

One example involves understanding of non-equilibrium quantum phases. This is especially challenging since, almost by definition, the equations of motion of an out-of-equilibrium system are constantly in flux. For instance, in the case of periodically driven (Floquet) systems, these equations of motion are periodic, but the non-equilibrium system is generically expected to absorb energy from the driving field (so-called Floquet heating) until it approaches a featureless infinite temperature state, thus preventing any nontrivial quantum ordering. Part of the success of experimentally realizing non-equilibrium phases of matter is owed to the theoretical development of strategies to prevent such Floquet heating (including most notably many-body localization; see Chapter 3 for additional discussion). One recent example of an intrinsically non-equilibrium phase realized in the laboratory is the discrete time crystal (see Box 4.2), whose ordering spontaneously breaks the time translation symmetry of the underlying drive. The period of the resulting discrete time crystal is quantized to an integer multiple of the drive period, and arises from collective synchronization. Another recent example involves experimental discovery of so-called quantum many-body scars, involving special slowly thermalizing trajectories in many-body Hilbert space of constrained, strongly interacting systems, which are accompanied by nonmonotonic slow entanglement growth (see Figure 4.4).

## BOX 4.2
## Time Crystal

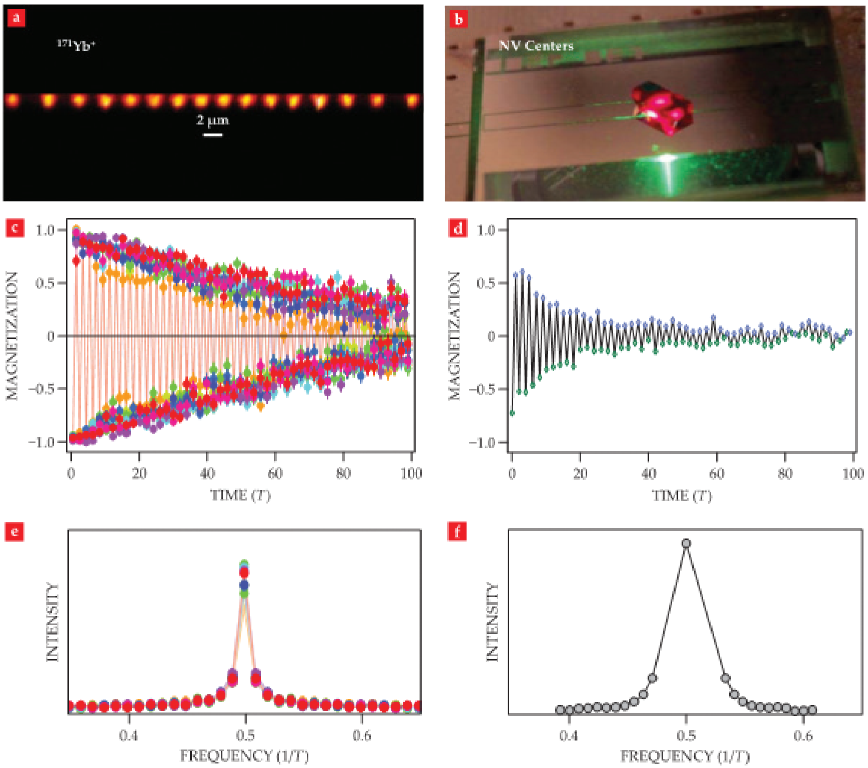

**FIGURE 4.2.1** Realization of discrete time crystalline order. The first signatures of discrete time-crystalline order were reported in two different effective spin systems. (a) A one-dimensional (1D) chain of trapped ytterbium ions. Each ion had an effective spin-1/2 state created from two of its hyperfine sublevels, and ion-ion interactions generated a lattice arrangement. (b) A three-dimensional (3D) ensemble of nitrogen-vacancy defects (NV centers) in diamond. The NV centers fluoresce red under green laser illumination. (c, d) Each system was driven by a Floquet sequence for about 100 cycles. (e, f) Fourier transforms of the measured magnetizations show sharp oscillations at half the cycle frequency 1/T, where T is the cycle period. SOURCE: Reprinted by permission from Springer Nature: J. Zhang, P.W. Hess, A. Kyprianidis, P. Becker, A. Lee, J. Smith, G. Pagano, I.-D. Potirniche, A.C. Potter, A. Vishwanath, N.Y. Yao, and C. Monroe, Observation of a discrete time crystal, *Nature* 543:217-220, 2017, https://doi.org/10.1038/nature21413, copyright 2017.

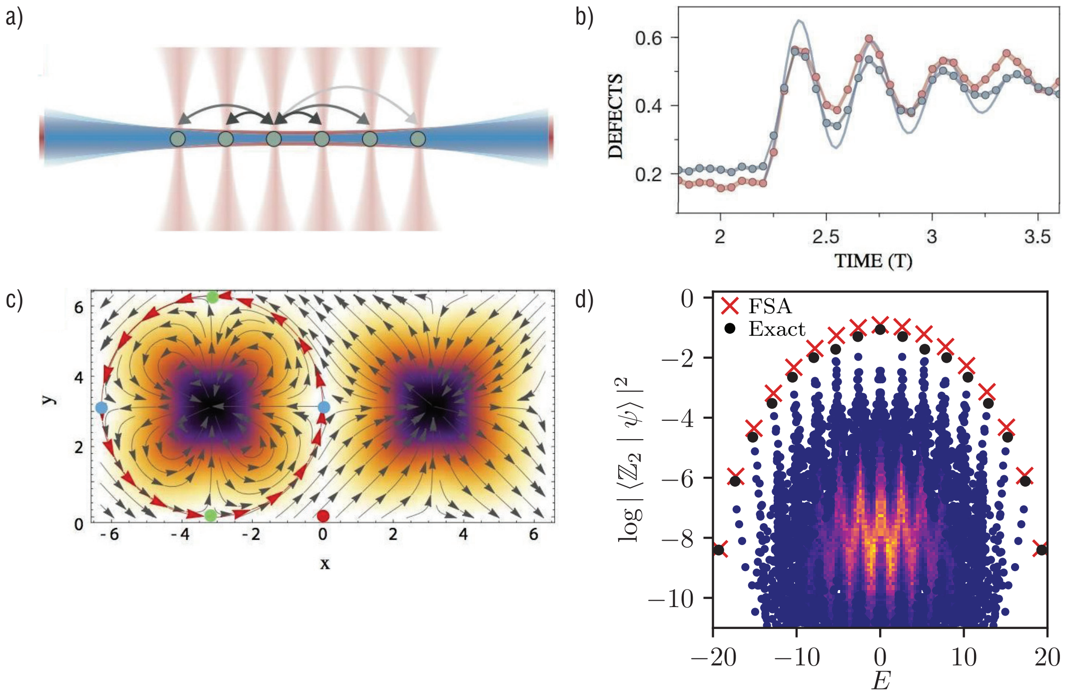

**FIGURE 4.4** Nonequilibrium quantum dynamics in 1D arrays of trapped neutral atoms. (a) Illustration of the experimental setup depicting interactions between atoms through excitation into Rydberg states. The position and the internal states of each atom can be controlled and manipulated by external lasers. (b) Experimental observation of surprising long-lived oscillations in a driven system initially prepared in the antiferromagnetic configuration. Figure shows density of defects associated with anti-ferromagnetic ordering as a function of time, indicating periodic oscillations of order parameter. (c) Theoretical analysis of the dynamics, based on a variational principle using minimally entangled Matrix Product States (parametrized by two variables x and y), yields effective equations of motions that support an isolated, periodic orbit (red circle). This orbit describes nonthermalizing dynamics, in contrast to the thermalizing behavior observed for other, generic initial conditions. (d) The spectrum of the system reveals that there exists a special subset of eigenstates that have remarkably high overlap with the initial ordered state; these states give rise to the so-called *many-body scarring* effect associated with stable trajectories in a complex many-body quantum system. The plot shows overlap between the initial, antiferromagnetically ordered state with all many-body eigenstates of the system as a function of their energy. SOURCE: (a-b) Reprinted by permission from Springer Nature: H. Bernien, S. Schwartz, A. Keesling, H. Levine, A. Omran, H. Pichler, S. Choi, A.S. Zibrov, M. Endres, M. Greiner, V. Vuletić, and M.D. Lukin, Probing many-body dynamics on a 51-atom quantum simulator, *Nature* 551:579-584, 2017, https://doi.org/10.1038/nature24622, copyright 2017. (c) W. Wei Ho, S. Choi, H. Pichler, and M.D. Lukin, Periodic orbits, entanglement, and quantum many-body scars in constrained models: Matrix product state approach, *Physical Review Letters* 122:040603, 2019, https://doi.org/10.1103/PhysRevLett.122.040603, copyright American Physical Society. (d) Reprinted by permission from Springer Nature: C.J. Turner, A.A. Michailidis, D.A. Abanin, M. Serbyn, and Z. Papić, Weak ergodicity breaking from quantum many-body scars, *Nature Physics* 14(7):745-749, 2018, https://doi.org/10.1038/s41567-018-0137-5, copyright 2018.

### From Many-Body Physics to Lattice-Gauge Theories and High-Energy Physics

During the past decade, the development of atomic quantum simulators has been mainly driven by the attempt to gain insight into strongly correlated many-body systems of condensed-matter physics. Physically interesting quantum many-body systems, which cannot be solved with classical simulation methods, have become accessible to analog or digital quantum simulation with cold atoms, molecules, and ions. In the future, quantum simulators may also enable us to address currently unsolvable problems in particle physics, including the real-time evolution of the hot quark-gluon plasma emerging from a heavy-ion collision or the deep interior of neutron stars.

The phenomena in condensed-matter and high-energy physics the committee wants to address are described by gauge theories, and the challenge is thus the development of quantum simulators for gauge, and in particular, lattice-gauge theories—that is, gauge theories discretized on a lattice. In particle physics, Abelian and non-Abelian gauge fields mediate the fundamental strong and electroweak forces between quarks, electrons, and neutrinos. In atomic and molecular physics, electromagnetic Abelian gauge fields are responsible for the Coulomb forces that bind electrons to atomic nuclei. In condensed-matter physics, besides the fundamental electromagnetic field, effective gauge fields may emerge dynamically at low energies. Examples of phenomena, which can be understood in a lattice gauge language include anyonic statistics of quasiparticles in quantum-Hall systems, or quantum spin liquids, which may arise in geometrically frustrated antiferromagnets. Furthermore, universal topological quantum computation is based on non-Abelian Chern-Simons gauge theories. Box 4.3 illustrates the basic features of lattice-gauge theories with the example of quantum spin-ice as a frustrated spin-model in condensed-matter physics, and 1D QED, the so-called Lattice Schwinger Model.

While quantum simulation of gauge theories is fundamental, it is challenging to implement lattice-gauge models with atomic setups (and other platforms). The Hamiltonians for gauge models to be realized in the atomic laboratories are complex (see, e.g., Figure 4.3.1b), and often do not have a natural counterpart in atomic lattice models—for example, the familiar Hubbard models with cold bosonic and fermionic atoms in optical lattices. Instead, these models are obtained only as emergent lattice-gauge models in atomic models—that is, as effective models in the low-energy sector with high-energy degrees of freedom integrated out. However, designing such effective Hamiltonians for analog quantum simulation comes at a price: not only is it nontrivial to engineer the required gauge-invariant Hamiltonian couplings from the available atomic resources, but also the resulting energy scales of these effective theories can be small, with corresponding stringent

## BOX 4.3
## Lattice-Gauge Theories in Condensed-Matter Physics and High-Energy Physics

The key feature of gauge theories is redundancy in our description of nature. In a theoretical formulation, this redundancy is reflected as a local symmetry, the so-called gauge symmetry, and there is an associated local conservation law (Gauss's law). Figure 4.3.1 illustrates the basic ingredients of Abelian lattice-gauge theories as quantum spin-ice taken from condensed-matter physics. In Figure 4.3.1(a), the magnetic moments (yellow arrows) of rare-earth ions are located on the corners of a pyrochlore lattice, which is a network of corner-sharing tetrahedra. They behave as almost perfect Ising spins and point along the line from the corner to the center of the tetrahedron, either inward or outward. Degenerate ground-state configurations obey the "ice rules," which enforce two spins pointing inward and two spins pointing outward at each vertex—that is, a Gauss's law. Figure 4.3.1(b) shows spin configurations allowed by Gauss's law for two-dimensional quantum spin ice.

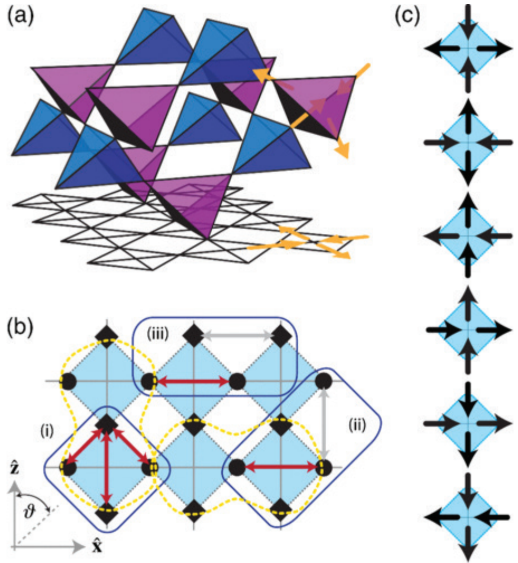

**FIGURE 4.3.1** Lattice-gauge theories and Gauss's law in condensed-matter physics. (a) In spin-ice materials, the magnetic moments (yellow arrows) of rare-earth ions are located on the corners of a pyrochlore lattice, which is a network of corner-sharing tetrahedra. They behave as almost perfect Ising spins and point along the line from the corner to the center of the tetrahedron, either inward or outward. Because of the different Ising axes of the spins, this results in an effectively antiferromagnetic interaction that is frustrated. (b) Projecting the 3D pyrochlore lattice onto a 2D square lattice yields a checkerboard lattice, where tetrahedrons are mapped onto crossed plaquettes (light blue). Interactions between two spins located on • or ♦ lattice sites have to be steplike (as a function of the distance) and anisotropic, and they require a bipartite labeling of the lattice sites. (c) Degenerate ground-state configurations of spins on a crossed plaquette. They obey the "ice rules," which enforce two spins pointing inward and two spins pointing outward at each vertex, reminiscent of Gauss's law in electrodynamics. SOURCE: *Phys. Rev. X* 4, 041037, 2014.

requirements for temperature and decoherence times in experiments. Numerous theory proposals have been made in recent years to implement analog quantum simulation of Abelian and non-Abelian lattice-gauge theories for spin models, and with fermionic and bosonic atomic mixtures in specially engineered lattice geometries. However, an experimental realization of analog quantum simulation of lattice-gauge theories remains an outstanding challenge.

Quantum simulation can be implemented not only as an analog simulation but also as a digital quantum simulation. For example, the time evolution generated by a (potentially complex) Hamiltonian can be decomposed into Trotter steps—that is, essentially using a universal quantum computer to propagate the quantum many-body problem. Real-time dynamics for a Lattice Schwinger Model has been studied with a trapped-ion quantum processor (see Figure 4.5). The committee emphasizes, however, that this programming of complex many-body dynamics on a universal quantum computer is expensive, and for present devices is restricted to a small number of qubits and Trotter steps (four qubits, and four Trotter steps). Scaling digital quantum computations and simulations to a large number of qubits, and in a fault-tolerant way, is again one of the outstanding challenges for the future.

There is a third method of quantum simulation of complex many-body problems: variational quantum simulation. Refer to the section "From Quantum Computers to Programmable Quantum Simulators" earlier in this chapter for a description of this technique.

## Applications to Quantum Chemistry

In the early 20th century, the new field of quantum chemistry was formed by the interaction of chemists, physicists, applied mathematicians, and computer scientists. One hundred years later, we have seen the birth of quantum information for quantum chemistry, building on discoveries at the nexus between modern theoretical physical chemistry and the new ideas emerging from quantum information theory and its foundations in quantum physics and computer science. For the past two decades, research has been focused on (1) elucidating the role of quantum information in molecular systems and using this to solve outstanding problems in chemistry, (2) re-envisioning quantum spectroscopy and control, and (3) constructing and utilizing quantum information processors and developing applications for these in chemistry.

Today, many theoretical/computational chemists rely on large computational packages such as GAMESS and GAUSSIAN and other software packages that in part employ extremely efficient Gaussian integral evaluations. To achieve chemical accuracy (1 kcal/mol or fewer) in a systematic way, they rely on using either variational expansion methods such as multi-configuration self-consistent field or

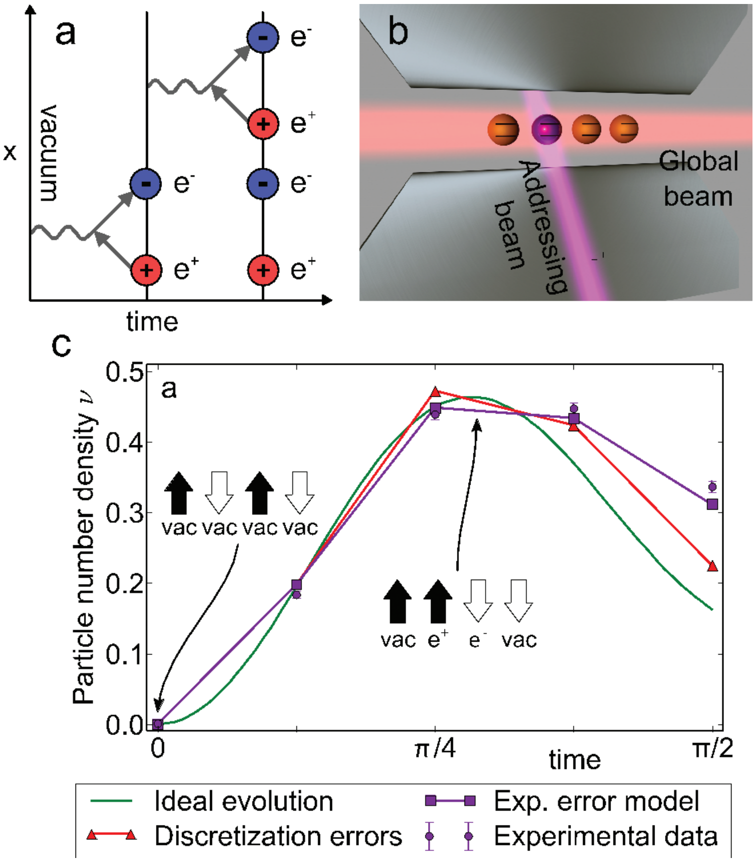

**FIGURE 4.5** Digital quantum simulation of the Lattice Schwinger Model as one-dimensional (1D) quantum electrodynamics (QED). (a) The instability of the vacuum due to quantum fluctuations is one of the most fundamental effects in gauge theories. The coherent real-time dynamics of particle-antiparticle creation is simulated by realizing the Schwinger Model (1D QED) on a lattice. (b) The experimental setup for the simulation consists of a linear Paul trap, where a string of $^{40}Ca^+$ ions is confined. The electronic states of each ion, depicted as horizontal lines, encode a spin $|\uparrow\rangle$ or $|\downarrow\rangle$. These spin states can be manipulated using laser beams. In the quantum simulation, electron and positron configurations on the lattice are encoded in spin configurations, and are propagated on the four-qubit ion-trap quantum computer for four Trotter steps (involving a total of 220 quantum gates). (c) Time evolution of the particle number density, $\nu$. The figure compares the ideal evolution under the Schwinger Model, the ideal evolution considering Trotter time discretization errors, and the experimental data and a model of it. NOTE: For details of the model and the definition of the symbols, see Martinez et al. (2016). SOURCE: Reprinted by permission from Springer Nature: E.A. Martinez, C.A. Muschik, P. Schindler, D. Nigg, A. Erhard, M. Heyl, P. Hauke, et al., Real-time dynamics of lattice gauge theories with a few-qubit quantum computer, *Nature* 534:516-519, 2016, https://doi.org/10.1038/nature18318, copyright 2016.

configuration interaction methods with large basis sets or perturbative expansions such as Coupled Cluster (e.g., CCSDT) and many-body perturbation theory such as MP3. Supplementing these methods, Density Functional Theory and to a lesser extent a variety of forms of quantum Monte Carlo have become popular in certain circles. Despite the progress in developing such electronic structure methods, many important problems in chemistry such as the prediction of chemical reactions and the description of excited electronic states, transition states, and ground states of transition-metal complexes that are essential for material design, although doable by these methods, remain challenging. The accuracy requirements for prediction (and identification) of spectra of atoms and molecules relevant to astrophysics are even more demanding (i.e., much better than 0.01 $cm^{-1}$ uncertainty in inverse wavelength). At present theorists are using a combination of empirical fitting methods and tuning molecular potential energy surfaces to fit spectra. Substantial improvements in the accuracy of ab initio calculations need to be achieved and represent an important challenge for the future.

Bringing techniques from quantum information into the picture may enable treatment of some of these hard problems. Based on the different variations of the phase estimation algorithm, mappings to Ising Hamiltonians, the variational quantum eigensolver (VQE), and other quantum simulation techniques, scientists have been able to obtain results with modest accuracy using up to six qubits on several experimental platforms (photonic quantum computer, NMR, ion trap, and superconducting-based qubits) for small molecules such as $H_2$, $BeH_2$, LiH, and $H_2O$. The big question is how to proceed to perform electronic-structure calculations for large chemical systems! Recently, Reiher et al. showed how quantum computers (with about 110 logical qubits) can be used to elucidate the reaction mechanism for biological nitrogen fixation in nitrogenase, by augmenting classical calculation of reaction mechanisms with reliable estimates for relative and activation energies that are beyond the reach of traditional methods. One can assume that treating complex chemical systems in the field of catalysis, drug design, cluster optimization, and so on will need at least hundreds of logical error-corrected qubits (thousands to millions of physical qubits!). To address these challenges, a number of exciting research directions are currently being explored. These include the following:

1. Developing hybrid quantum-classical algorithms: The initial development of VQE is a good example in this direction: one uses a quantum device to evaluate the expectation value of the objective function depending on parameters that are optimized through classical methods. See, for example, Box 4.1, earlier in this chapter.
2. Developing quantum machine learning: Combining machine learning techniques with quantum algorithms. The initial development of the Boltzmann machine for quantum simulations is a good example in this direction.

3. Designing quantum algorithms relevant to chemistry based on *d*-level systems qudits (where "d" is an integer greater than two) instead of qubits. Initial ideas of exploiting a natural mapping between vibrations in molecules and photons in waveguides is a good example of simulating the vibrational quantum dynamics of molecules using programmable photonic chips based on qudits.
4. More broadly exploiting quantum information ideas for *chemistry:* This has led to progress in quantifying entanglement in chemical reactions and complex biological systems. However, how to measure entanglement between electrons in chemical reactions is still a challenge. Also, how the quantum resources of interference, superposition, and entanglement can assist in quantum control of chemical reactions is still at an early stage.

## BELL INEQUALITIES, QUANTUM COMMUNICATION, AND QUANTUM NETWORKS

### From Bell Inequalities to Quantum Communication

Quantum theory predicts that reality is not nearly as simple as one might have imagined. In particular, it predicts that physical quantities observable in experiments do not have values until they are measured. Einstein identified, and famously objected to, this feature of the theory. However John Bell devised an experimental "Bell inequality" test that only the quantum theory could pass and any classical theory (in which observables have values before they are measured) must fail. In addition to being of profound importance to our understanding of the nature of physical reality, Bell inequalities are now becoming critical system engineering tests that certify a computer is truly quantum, certify true random number generation, and certify the security of encryption and communication.

Experimental tests of Bell inequalities have played an important role in the emergence of quantum information, by drawing the attention of physicists to the revolutionary character of entanglement. One can find a witness of this role in the paper by Feynman considered a founding paper of quantum computing,[3] in which he writes: "I've entertained myself always by squeezing the difficulty of quantum mechanics into a smaller and smaller place, so as to get more and more worried about this particular item. It seems to be almost ridiculous that you can squeeze it to a numerical question that one thing is bigger than another. But there you are—it is bigger than any logical argument can produce." Although he does not give any reference, Feynman clearly refers to Bell inequality violations.

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[3] R.P. Feynman, Simulating physics with computers, *International Journal of Theoretical Physics* 21:467-488, 1982.

Bell inequalities[4,5] refer to the strong correlations between measurements on two quantum objects initially prepared together in an entangled state—for instance, polarization measurements of two photons emitted in opposite directions. The violation of Bell inequalities means that it is impossible to understand these correlations by invoking unknown common properties, properties not part of the standard quantum formalism (e.g., local supplementary parameters or "hidden variables"), determined at the preparation and carried along separately by each subsystem. Such models, widely used in classical science, allow one to explain, for instance, correlations of some diseases of identical twins, who carry along the same set of chromosomes. Renouncement of the corresponding worldview, known as "local realism" and advocated by Einstein, was considered surprising enough to demand experimental tests. In fact, situations in which Bell inequalities are predicted to be violated by quantum systems are so rare that specific experiments had to be designed to perform the tests. And some now widely used quantum technologies, such as efficient sources of pairs of entangled photons, were developed to make these tests possible.

Almost immediately after the first convincing tests, in the 1970s, showing that quantum mechanics remains valid even in extreme situations where Bell inequalities are violated, questions were raised about possible loopholes in the tests, with two main targets: (1) the detection loophole—that is, the fact that detectors with limited sensitivity, which miss a significant fraction of the photons, leave open the possibility of some classes of local supplementary parameters; and (2) the locality loophole—that is, the fact that in order to prevent any possible unknown interaction between the separated objects, one should make relativistically independent measurements, in which the settings of the instruments and the measurements themselves are separated by a space-like interval, so that no interaction obeying the impossibility to propagate faster than light could interfere with the test. The locality loophole, the most important according to Bell, was addressed as early as 1982, and its closure was confirmed by several later experiments. The detection loophole, on the other hand, could be closed only with the development of new detectors with efficiencies close to 100 percent, in the 2010s. Closing the two loopholes in the same experiment demanded a new generation of experimental setups, and eventually happened in 2015. After decades of discussions, controversies, and experimental advances, it is hard not to admit that entanglement is real, and as weird as Einstein, Schrödinger, Feynman, and others thought it to be.

Beyond their role in the emergence of quantum information, Bell inequalities are directly involved in quantum cryptography, and specifically quantum key

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[4] J.S. Bell, On the Einstein-Podolsky-Rosen paradox, *Physics* 1:195-200, 1964.

[5] J.S. Bell, *Speakable and Unspeakable in Quantum Mechanics*, Cambridge University Press, 2004 (revised edition).

distribution (QKD). The basic problem addressed by QKD is to distribute to two spatially separated partners, Alice and Bob, two identical random sequences of zeros and ones. Alice and Bob will then use them as a key to encode and decode messages. The protocol, known as a "one-time pad," is mathematically proven secure, provided that the key is used only once, for a message not longer than the key. One of the methods used to generate safely, at a distance, the two identical random sequences of zeros and ones, is based on pairs of entangled photons, which yield random but identical results if Alice and Bob choose identical settings for their measurement devices. The whole protocol demands that Alice and Bob choose at random various settings among a small list of predetermined values. After completing the measurements, they exchange information, on a public channel, about what were the chosen settings, and about some results. This allows them to select the cases of identical settings and to identify the identical keys, but other settings allow them to make a test of Bell inequalities. If they find a violation, they can be sure that there is no eavesdropper (Eve) on the line, spying on their exchange of quantum information.

Many sophisticated protocols have been elaborated based on the idea that a Bell test is a way to check whether information could be obtained by a spy. In principle, such a verification is device independent, meaning that it suffices to find a violation of a Bell inequality to be sure that no information has been obtained by Eve, independently of a detailed knowledge of the employed apparatuses. Surprisingly, this kind of idea also applies to other protocols, such as the famous BB84 protocol, or continuous variables protocols, which do not use sources of entangled photon pairs. Many sophisticated protocols have been developed to take account of the imperfections of real devices in the search for practical device-independent QKD (meaning that the performance of the devices is such that they can be certified, via Bell inequality tests, safe to use even if provided by a third party). One can expect that these ideas will yield realizations of quantum cryptography devices even safer than the systems already commercially available.

One could consider these efforts to be pointless, since we have today classical cryptographic protocols, for instance the famous Rivest-Shamir-Adleman (RSA) cryptosystem, which were considered safe until recently. But we also know that RSA can be broken by Shor's algorithm on a quantum computer, or could be broken if an adversary would find a mathematical algorithm for a classical computer allowing that individual to speed up the decomposition of a large number into its prime factors, or if the adversary had computers more powerful than ours. This may well happen in the future, which means that present encrypted messages, saved blindly today, could be deciphered a few years from now. There are many domains, from diplomacy to industrial processes, where this would be detrimental even with long delays. In contrast, intercepted messages encrypted with quantum cryptography promise to remain impossible to decipher forever, or at least as long as the basic laws of quantum physics remain valid. This is not a small advantage.

Among the advances in quantum technologies stimulated by the loophole-free tests of Bell inequalities, one in particular deserves special mention: the entanglement of two quantum bits separated by more than 1 km. Although the present entanglement rate is extremely low, it demonstrates the possibility to entangle quantum memories at a significant distance. Such memories will be essential in future quantum networks.

Nevertheless, a major problem remains to be solved: how to create and maintain entanglement at large distance, say, more than 50 km. At such a distance, even the best optical fibers have too strong attenuation, and it would be necessary to rejuvenate a pair of entangled photons with a series of QRs spaced at shorter distances along the way. Although several setups have been proposed, and some of their elements have been experimentally demonstrated, no practical QR exists today. Various systems are under study, in AMO physics and in condensed-matter laboratories, as described in the following section. For the time being, expedients must be used. One approach consists of building every 50 km a "trusted node"—that is, a building controlled by trusted guards, where the quantum information is converted to classical information and then resent in a rejuvenated quantum form. While this approach can possibly be used for some specific applications, over limited distances, it does not provide a true quantum security guarantee, does not allow for the distribution of superposition states, and can hardly be generalized to the scale of the world. More interestingly, pairs of entangled photons sent from a satellite (acting as a trusted node) have been distributed over distances on the order of 1,000 km,[6] since they suffer from absorption only in the atmospheric part of the photon trajectories. This approach is currently limited by several factors, including low quantum key generation rate, and a number of major engineering challenges that must be overcome to achieve large-scale practical application.

Another application of the Bell tests, less cited but important, is the validation of a genuine random number generator (RNG). A possible definition of a genuine RNG is one whose output cannot be known by anybody before it is delivered. Measurements on only one of the components of an entangled pair fulfill that condition, if a Bell test shows a violation of Bell inequalities, since then we know that there cannot be a local supplementary parameter determining the result of the measurement. This is another example of a device-independent certification based on the Bell inequalities test.

## Long-Distance Quantum Communication and Applications of Distributed Entanglement

As mentioned above, efficient quantum communication over long distances (≥1,000 km) remains an outstanding challenge due to attenuation and operation

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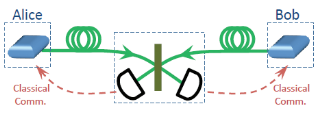
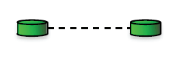
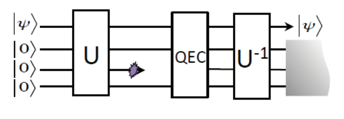
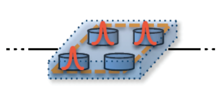
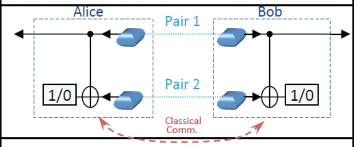
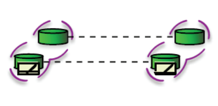
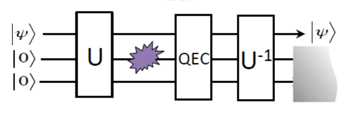
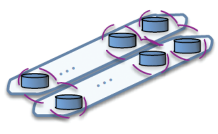
[6] J. Yin, Y. Cao, Y.-H. Li1, S.-K. Liao, L. Zhang, J.-G. Ren, W.-Q. Cai, et al., Satellite-based entanglement distribution over 1200 kilometers, *Science* 356:1180-1184, 2017.

errors accumulated over the entire communication distance. To overcome these challenges, QRs have been proposed for fiber-based long-distance quantum communication. The essence of QRs is to divide the total distance of communication into shorter intermediate segments connected by QR stations, in which loss errors and operation errors can be suppressed, by applying error detection (e.g., heralded entanglement generation and purification) or even error correction operations. Based on the methods adopted to suppress loss and operation errors, various QRs can be classified into three different generations (types), as shown schematically in Figure 4.6. These various QRs can significantly reduce the temporal resource overhead associated with extending the distance of the generated entanglement, from exponential to polynomial or even poly-logarithmic scaling with distance, while maintaining a reasonable physical resource requirement.

The capability of generating long-distance entanglement with QRs opens many new promising applications. Global-scale privacy-related protocols can be implemented, such as sharing of classical or quantum secrets, schemes for verifiable multiparty agreement, anonymous transmission, secure delegated quantum computing using network-based untrusted servers, and even blind computation wherein algorithms are performed directly on encrypted data. In addition, other related interesting applications have been proposed outside the domain of cryptography. For example, we can build long-baseline optical telescopes to improve astronomical observations and improve the synchronization and security of quantum networks of clocks.

To physically implement QRs, it will be advantageous to take a hybrid approach, as other physical platforms might provide better quantum memory and quantum gates than photonic systems. The hybrid approach often requires the quantum system to have (1) a quantum interface to reliably couple to the fiber optical modes, (2) good heralded quantum memory for storage and entanglement purification, and (3) the capability of quantum gates for quantum error detection/correction. Note that the quantum memory requirement varies for different generations of QRs. The implementation of quantum gates can be nondeterministic—for example, operations based on heralded partial Bell measurements. Recently, there have been significant advances in developing such hybrid quantum systems, based on trapped ions, neutral atoms, color defect centers, quantum dots, rare-earth ions, superconducting devices, and so on.

The outstanding challenge is to develop a hybrid quantum system that can simultaneously fulfill all these requirements with high fidelity and efficiency. There is now a broad effort across various promising physical platforms to first demonstrate QRs. The trapped-ion platform (with good memory and reliable gates) has recently improved the optical coupling efficiency by orders of magnitude, so that it can generate entanglement faster than the observed decoherence, overcoming the resource scaling requirement for quantum networks. Atomic ensembles with Rydberg

| Errors | Approaches | Examples | Schematics | 1G | 2G | 3G |
|---|---|---|---|---|---|---|
| Loss Error | Heralded Entanglement Generation (HEG) |  |  | ✓ | ✓ | |
| | Quantum Error Correction (QEC) |  |  | | | ✓ |
| Operation Error | Heralded Entanglement Purification (HEP) |  |  | ✓ | | |
| | Quantum Error Correction (QEC) |  |  | | ✓ | ✓ |

**Elements:**

- Remotely entangled qubit
- Flying qubit (photons)
- CNOT gate
- Qubit in an encoded block
- Measurement (X/Z)
- Teleportation-based Error Correction

**FIGURE 4.6** A list of methods to correct loss and operation errors in quantum repeaters (QRs). QRs are categorized into three generations (denoted 1G, 2G and 3G respectively), depending on the methods used to correct the errors. Loss error can be suppressed by either heralded entanglement generation (HEG) or quantum error correction (QEC). During HEG, quantum entanglement can be generated with techniques such as two-photon interference conditioned on the click patterns of the detectors in between. Loss errors are suppressed by repeating this heralded procedure until the two adjacent stations receive the confirmation of certain successful detection patterns via two-way classical signaling, while simultaneously storing successfully entangled pairs. Alternatively, one may encode the logical qubit into a block of physical qubits that are sent through the lossy channel and use quantum error correction to restore the logical qubit with only one-way signaling. Quantum error correcting codes can correct no more than 50 percent loss rates deterministically due to the no-cloning theorem. To suppress operation errors, one may use either heralded entanglement purification (HEP) or QEC as mentioned earlier. In HEP, multiple low-fidelity Bell pairs are consumed to probabilistically generate a smaller number of higher-fidelity Bell pairs. Like HEG, to confirm the success of purification, two-way classical signaling between repeater stations for exchanging measurement results is required. Alternatively, QEC can correct operation errors using only one-way classical signaling, but it needs high fidelity local quantum gates. SOURCE: S. Muralidharan, L. Li, J. Kim, N. Lütkenhaus, M.D. Lukin, and L. Jiang, Optimal architectures for long distance quantum communication, *Scientific Reports* 6:20463, 2016, https://doi.org/10.1038/srep20463.

interactions not only have good optical coupling, but also Rydberg-induced photon-photon interactions for deterministic gates to enhance the efficiency of QR nodes. Various quantum transducers for microwave-optical conversion are actively being pursued using various hybrid systems, which will extend superconducting quantum information processing capability from microwave to optical photons for quantum networks. Nanophotonic devices coupled to cold atoms or atom-like solid-state quantum emitters can efficiently guide the emitted photons to optical fibers with extremely high efficiency (>95 percent), enabling access to individual rare-earth ion quantum memories, demonstrated at Princeton University, or even providing controlled interactions between pairs of color centers, demonstrated at Harvard. In particular, integrated quantum network nodes combining all necessary ingredients have been demonstrated recently using silicon-vacancy centers in diamond. Most recently, this system was used by the Harvard University-Massachusetts Institute of Technology collaboration to demonstrate memory-enhanced quantum communication. Specifically, a single solid-state spin memory integrated in a nanophotonic diamond resonator was used in a proof-of-concept experiment to implement asynchronous Bell-state measurements, a key element of QR. This enabled a four-fold increase in the quantum communication rate of over the loss-equivalent direct-transmission method while operating megahertz clock rates. In the coming decade these approaches will likely result in realization and testing of medium-scale, functional quantum network prototypes that extend the range of quantum communication.

## QUANTUM INFORMATION SCIENCE FOR SENSING AND METROLOGY

### Realization of Spin Squeezing

Many precision measurements in atomic physics are carried out in the form of a frequency measurement of the phase evolution speed between two atomic states (see also Chapter 6). When the measurement is performed with many independent particles to increase the signal-to-noise ratio, the precision increases as the square root of the particle number, a situation referred to as the standard quantum limit (SQL). The SQL can be overcome by using many-atom entangled states to perform the measurement. With suitably chosen states, the measurement precision can be significantly better than the SQL, and in principle approach the Heisenberg limit, where the precision improves linearly with the particle number. Highly useful entangled states are squeezed spin states (SSSs), in which the uncertainty in one variable of interest is reduced at the expense of another variable that does not affect the measurement precision to lowest order. SSSs can be directly used as input states to a standard metrology procedure (such as Ramsey sequence; see Figure 4.7), yielding lower quantum noise than a corresponding sequence with an

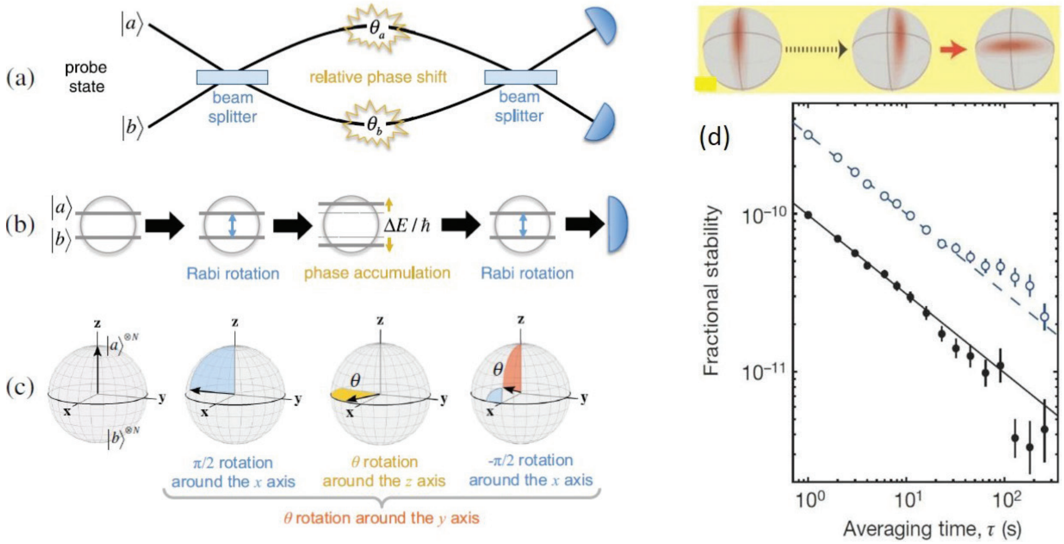


**FIGURE 4.7** Ramsey sequence and interferometer. (a) A Mach-Zehnder interferometer measures interferometrically a phase difference between two paths. In a Ramsey interferometer (b), a resonant Rabi rotation creates a balanced superposition between two internals states whose relative phase is measured. (c) Equivalent representation of Mach-Zehnder and Ramsey interferometer operations as rotations of the collective spin on the generalized Bloch sphere. (d) Squeezed spin states (SSSs) are used for realizing better phase resolution in a Ramsey sequence than an unentangled coherent spin state (CSS) and clock stability comparison between a CSS (open circles) and an SSS (solid circles), showing that the SSS reaches a given precision 11 times faster than a CSS. SOURCE: Reprinted figure with permission from L. Pezzè, A. Smerzi, M.K. Oberthaler, R. Schmied, and P. Treutlein, Quantum metrology with nonclassical states of atomic ensembles, *Reviews of Modern Physics* 90:035005, 2018, https://doi.org/10.1103/RevModPhys.90.035005, copyright by the American Physical Society.

unentangled coherent spin state (CSS). In Bose-Einstein condensates, SSSs can be prepared using state-dependent collisions. Another possibility, more suitable for precision measurements, is optical preparation, in which a mode of a light field acts as an intermediary that creates an effective spin-dependent atom-atom interaction.

To make the interaction as coherent and strong as possible, an optical resonator enclosing the ensemble can be used. In this way, spin squeezing approaching 20 dB has been realized. This number corresponds to a reduction of the variance by a factor 100 below the SQL, which, under ideal circumstances, would enable a reduction of the measurement time to reach a given precision by the same factor.

SSSs can in principle be used to improve any quantum measurement based on interference—for example, Ramsey-type measurements. A particularly interesting possibility is the application to optical-lattice clocks, that are already achieving precision at the low $10^{-17}/\mathrm{Hz}^{1/2}$ level at JILA and NIST, and fractional accuracies at the $10^{-18}$ level, and that are operating at or near the SQL. Here SSSs could usher in a new generation of clocks, where many-body entangled states can further increase the precision by one or two orders of magnitude, leading to, for example, gravitational-red-shift sensitivity at the millimeter scale. Other promising applications of SSSs include atom interferometry to achieve unprecedented signal-to-noise ratio for precision tests and measurements of fundamental constants.

### New Applications of Quantum Sensing

In recent years, solid-state atom-like quantum systems have attracted intense interest as precision quantum sensors with wide-ranging applications in both the physical and life sciences. Most prominently, nitrogen-vacancy (NV) color centers in diamond provide an unprecedented combination of nanoscale spatial resolution and sensitivity to electromagnetic fields and temperature, while operating over a wide range of temperatures from cryogenic to well above room temperature in a robust, solid-state system. Importantly, since NV centers are atomic-size defects and can be localized very close to the diamond surface, they can be brought to within a few nanometers of the sample of interest, greatly enhancing the sample's magnetic or electric field at the position of the NV sensor and enabling nanometer-scale spatial resolution. For magnetic field sensing, one optically measures the effect of the Zeeman shift on the NV ground-state spin levels. Similarly, NV-diamond can provide nanoscale electric field sensing via a linear Stark shift in the NV ground-state spin levels induced by interactions with the crystalline lattice and can provide nanoscale temperature sensing via a change in the zero-magnetic-field splitting between the NV spin levels. In addition, NV-diamond has other enabling properties for both physical and life science applications, including the following: fluorescence that typically does not bleach or blink; ability to be fabricated into a wide variety of forms such as nanocrystals, atomic force microscope tips, and bulk chips with NVs a few nanometers from the surface or uniformly distributed at high density; compatibility with most materials (metals, semiconductors, liquids, polymers, etc.); benign chemical properties; and good endocytosis with no known cytotoxicity for diamond nanocrystals and other structures used in sensing and imaging of living biological cells and tissues.

Applications of NV-diamond quantum sensors are rapidly advancing and diversifying, with translation of the technology into other fields accelerating and commercialization under way. Some recent highlights and their future potential are outlined here. NMR detection of a single protein and MRI of a single proton with angstrom resolution may lead to structure determination of individual proteins and other materials of interest with atomic-scale resolution (see Box 4.4). Noninvasive sensing and imaging of biomagnetism in living cells and whole animals with submicron resolution—for example, see Figure 4.8—provides a powerful new platform for studies in cell biology, genetics, brain function and disease, as well as lab-on-a-chip bioassays. In vivo nanodiamonds, which have been used to map temperature and

## BOX 4.4
## Single-Cell Quantum Diamond NMR/MRI

Recent advances in quantum diamond sensors have realized high-resolution NMR spectroscopy on samples comparable to the volume of single biological cells (Figure 4.4.1)[1] with sensitivity in such volumes to millimolar concentrations of physiologically relevant molecules.[2] They were also utilized to demonstrate NMR spectroscopy of individual proteins.[3] In the next few years, quantum diamond sensors may be integrated with silicon CMOS technology, microcoils to provide strong pulsed magnetic field gradients for MRI, and microfluidics. The resulting "on-chip" quantum diamond NMR/MRI could enable label-free sensing of biomarkers, single-cell metabolomics for quantitative cell biology and cell-based drug screening, and functional and structural MRI of biological tissues and organisms with subcellular resolution, thus providing a revolutionary new tool to chemical and biological scientists.

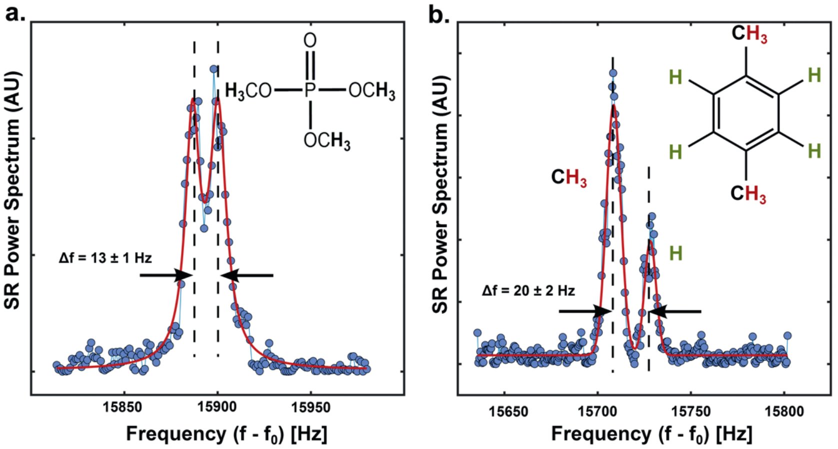


**FIGURE 4.4.1** Quantum diamond NMR spectroscopy of picoliter volume samples. (a) NV-NMR spectrum of trimethyl phosphate with splitting Δf = 13 ± 1 Hz due to J-coupling between the central $^{31}P$ nucleus and methyl protons. (b) NV-NMR spectrum of xylene with splitting Δf = 20 ± 2 Hz due to chemical shifts associated with two proton positions. NOTE: See D.R. Glenn, D.B. Bucher, J. Lee, M.D. Lukin, H. Park, and R.L. Walsworth, High-resolution magnetic resonance spectroscopy using a solid-state spin sensor, *Nature* 555:351-354, 2018; I. Lovchinsky, A.O. Sushkov, E. Urbach, N.P. de Leon, S. Choi, K. De Greve, R. Evans, et al., Nuclear magnetic resonance detection and spectroscopy of single proteins using quantum logic, *Science* 351(6275):836, 2016.

chemical changes in living human cells, have the potential for guiding thermoablative therapy for tumors and other lesions, and in the longer term may be used to monitor and even repair in vivo damage at the cellular and molecular level. Mapping of heterogeneous magnetic materials within primitive meteorites and early Earth rocks (>4 billion years old) with micron resolution is already providing key advances in the understanding of the formation of the solar system and Earth's geodynamo.

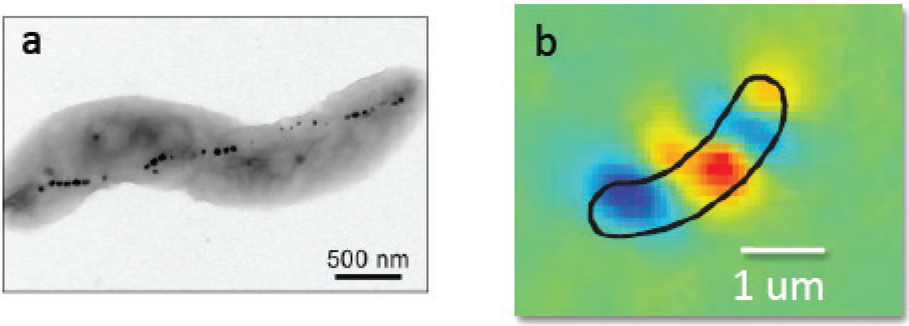


**FIGURE 4.8** Application of NV-diamond magnetic imaging to biology. (a) Transmission electron microscope (TEM) image of a magnetotactic bacterium (MTB). Magnetite nanoparticles in the magnetosome chain appear as spots of high electron density. (b) NV-diamond magnetic image of one MTB on the surface of the diamond chip, showing magnetic field patterns produced by the magnetosome with subcellular (400 nm) resolution. Cell outline (in black) is from a bright-field optical image of the MTB. Wide-field magnetic images of many living MTB in a population provide new biological information, such as the distribution of magnetic moments from individual bacteria in a particular MTB species. SOURCE: Adapted from D. Le Sage, K. Arai, D.R. Glenn, S.J. DeVience, L.M. Pham, L. Rahn-Lee, M.D. Lukin, A. Yacoby, A. Komeili, and R.L. Walsworth, Optical magnetic imaging of living cells, *Nature* 496(7446):486-489, 2013.

Similarly, imaging patterns of nanoscale magnetic fields is being successfully applied to a wide variety of advanced materials such as magnetic insulators undergoing spin injection, skyrmions, graphene, spin-torque oscillators, and canted antiferromagnets. This method may fill a critical technical need in the exploration and targeted development of smart materials for challenges in energy, the environment, information processing, and more. Recent work has also realized discrete time crystals in NV-diamond: this new form of matter may enable further advance in NV-diamond sensors by greatly extending the coherence time of dense NV ensembles. In addition, robust bulk diamond and nanodiamond sensors are being developed for extreme environments, which could provide unique tools for sensing buried ordinance and natural resources, as well as navigation, including underground, deep underwater, in conditions of extreme heat, radiation, pressure, and so on.

## GRAND CHALLENGES AND OPPORTUNITIES

### Grand Challenge: Realization of Large-Scale Quantum Machines and Networks

How do we build nearly perfect large-scale quantum machines out of a collection of imperfect parts? How do we nearly perfectly control these systems with imperfect controllers? The quantum states that give quantum machines their extraordinary powers are at the same time much more fragile than the states of classical machines. Furthermore, if we measure a quantum state, the very act of observation "collapses" that state. Thus, the task of fault-tolerant design is vastly more subtle and challenging than it is in traditional classical systems design. It is a remarkable fact that, with certain assumptions on the noise and error model, it is mathematically proven that fault tolerance is possible in principle. For quantum computing, this can be achieved by creating logical qubits that encode quantum information in entangled states of multiple physical qubits. To drive down the error rate, one can concatenate this procedure by building higher-level logical qubits from groups of lower-level logical qubits. Under concatenation, the error rate falls extremely rapidly. Unfortunately, the count of hardware parts rises exponentially with concatenation depth. The technological challenge at this stage of development is that we neither have access to exponentially large numbers of high-quality components nor the ability to control and measure them. It is possible that this challenge can be met head on through engineering, but an important intellectual challenge is to develop completely new ideas that will allow us to avoid the hardware count explosion and achieve practical fault tolerance in a manner that is much more "hardware efficient."

A related aspect of this grand challenge is the problem of navigating inside the enormous state space of quantum machines, measuring and controlling where the system is in this space and verifying that the quantum error-correction protocols and other processes are working as planned. In addition to Hamiltonian engineering, one must be able to control and engineer the dissipation in the system. Naively, dissipation is bad for quantum coherence, but new ideas and experiments are beginning to appear for using dissipation to stabilize and enhance coherence.

A third aspect is to connect quantum machines through quantum networks and to invent hybrid systems for transduction between different hardware platforms and signal modalities. For example, cryogenic superconducting microwave quantum circuits offer great advantages for universal control of complex photon states, while fiber optics offers the ability to transmit information over large distances at room temperature. In the past decade, promising first steps were taken toward transducers that can reversibly and noiselessly convert quantum information across the five-orders-of-magnitude frequency gap between the optical and microwave domains, but much remains to be done in the next decade. At the same time, recently demonstrated techniques for efficient interfacing between single photons and long-lived memories associated with spin states of individual quantum emitters will need to be developed and deployed for realization and testing of quantum networking protocols.

### Grand Challenge: Applications of Large-Scale Quantum Machines

Experimental efforts to manipulate large-scale quantum systems are achieving steadily improving results: systems involving approximately 100 strongly interacting, controllable quantum particles with large-scale entanglement are becoming an experimental reality. What can such quantum machines do both in principle and in practice? Can they provide a useful quantum advantage for real-world problems in areas such as computation, simulation, and communication? For example, even though recent advances already allow for unprecedented new insight into the physics of complex quantum many-body systems, it currently remains an open question if, and to what extent, large-scale quantum computers can be used to obtain meaningful speed-up for any practically relevant tasks apart from Shor's factoring algorithm. At the same time, while it is well-known that networks of quantum systems can potentially be used for nonlocal distribution of quantum entanglement, it is currently unclear how to implement any practically relevant applications beyond quantum key distribution, and to what extent they might work without error correction.

Addressing these exciting challenges will likely require coordinated effort across several subfields of physics, computer science, mathematics, chemistry, engineering, and materials science. New, efficient quantum algorithms for solving scientific and computational problems need to be developed and adopted for specific hardware implementations. Hybrid approaches combining state-of-the-art classical and quantum computational approaches also need to be explored. Most importantly, advances in building quantum machines should allow researchers to implement and test novel quantum algorithms for diverse scientific applications, and to explore practical methods for quantum error correction and fault tolerance. They could enable the first realizations and tests of quantum networks with applications to long-distance quantum communication and nonlocal quantum sensing.

### Grand Challenge: New Fundamental Science with Programmable Many-Body Systems and Quantum Simulators

The fact that the number of possible quantum states of a system grows exponentially with system size presents enormous challenges for the use of conventional computers to carry out numerical predictions of the properties of many-body systems and lattice-gauge theories of interest in condensed-matter, nuclear, and high-energy physics. We are just entering an exciting new era in which programmable quantum simulators are beginning to be used to elucidate the properties of important models and make new discoveries of great interest in these fields.

How do we make these quantum simulators fully programmable, large-scale, and also very high-fidelity (e.g., through quantum error correction and fault-tolerant quantum gate operations)? Quantum simulators offer the advantage of extraordinary experimental access through direct measurement techniques to the quantum state of the system being simulated. In particular, they allow one to measure the most fundamental properties of quantum many-body systems such as quantum entanglement and to explore fundamentally new phenomena away from equilibrium. However, many-body systems can be characterized not only by local order parameters that are easily measurable, but often by subtle nonlocal many-body correlations associated with hidden underlying characteristics—for example, the correlations that are associated with spin liquids. Much more work remains to be done to develop measurement techniques for these important but subtle quantities. Efforts combining the most advanced quantum and classical methods (such as those combining quantum simulators and classical and quantum machine learning) should be pursued.

As discussed further in Chapter 7, AMO physics produces new tools and measurement techniques that have broad impact in other fields of fundamental science as well as practical applications with economic impact. In particular, quantum matter and quantum sensors are playing an important role in the elucidation of new science in biology, medicine, cosmology, astrophysics, condensed-matter, geophysics, and other fields. The next decade will bring numerous additional opportunities for new science as well as new near-term applications.

### Quantum Information and AMO Physics: New Opportunities

The above considerations, consistent with *Quantum Computing,*[7] make it clear that despite major progress across several disciplines of physical, engineering, and computer science, the field of quantum information science and engineering is still in its early stages of development, with major outstanding challenges not only involving practical realization and applications of large-scale quantum machines, but of fundamental science as well. It is clear that AMO systems, methods, and techniques are uniquely suited to addressing these challenges in the coming decade, and will likely play a pivotal role in both basic science explorations and developing the first applications of quantum machines. The key distinguishing feature of AMO systems is a combination of an excellent degree of coherence and well-developed quantum control techniques that can be directly extended to medium-scale systems involving tens to hundreds of identical qubits without need for complex quantum error correction. In the coming decades, these systems and techniques should allow researchers to explore classically intractable problems in quantum dynamics, explore outstanding questions in physics of high-temperature superconductivity and in spin liquids, allow realization and testing of quantum optimization algorithms, and investigate hardware-efficient approaches to quantum error correction.

To support this assessment, the committee provides a brief summary of the most recent developments in the field, described in this chapter, that have occurred

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[7] National Academies of Sciences, Engineering, and Medicine, 2019, *Quantum Computing: Progress and Prospects*, The National Academies Press, Washington, DC.

since *Quantum Computing* was published in 2019, and the corresponding near-term opportunities that they open up.

Strings of trapped ions represent both a leading platform for universal quantum computation, and as a programmable analog quantum simulator. Experimentally, system sizes of 53 qubits have been built. Gate fidelities have improved to 99.9(1) percent, and operating speeds have increased to the microsecond scale. A central issue is scalability, and going from 1D to 2D ion-trap arrays. These advances in ion-trap quantum computing have enabled the implementation of a plethora of routines and algorithms. This includes repetitive error correction and encoding and operations in topological codes. With increasing numbers of qubits, routines are required to characterize, verify, and validate the performance of ion-trap devices. Prominent examples for such verification routines with trapped ions are scalable benchmarking, scalable tomography, and methods that work with incomplete data. On the quantum computing side, this provides a basis for the implementation of numerous algorithms and digital simulations such as Shor's algorithm, Bernstein-Vazirani, and the Hidden Shift algorithm. Furthermore, ion-trap quantum computer architecture has been used to implement digital quantum simulation. Particularly promising are variational quantum algorithms for quantum chemistry, and the recent implementation of variational quantum simulation of ground and excited states of lattice models. As discussed earlier in Box 4.1, this latter experiment demonstrated verification—that is, an error bar for variational energies was computed on the quantum machine.

Rydberg atom arrays emerged, based on the experiments carried out over the past 2 years, as a leading platform for quantum information processing and simulations. As discussed in the section "Controlled Many-Body Systems for Quantum Simulations," specific highlights include realization of a programmable quantum spin model with tunable interactions and system sizes of up to 51 qubits, and its use for probing the Kibble-Zurek mechanism, quantum critical dynamics, topological physics, discovery of quantum many-body scars, and, most recently, realization of a 20-atom GHZ state, the largest GHZ state demonstrated to date. This approach opens up unique opportunities for realizing deep quantum circuits with coherent systems consisting of hundreds of qubits in two or three spatial dimensions, with applications ranging from testing quantum algorithms and exploring efficient approaches for quantum error corrections, to realization of quantum machine learning models and generation of large-scale entangled states for quantum metrology. In particular, programmable quantum simulators based on trapped ions and neutral atoms hold great promise for simulating complex systems ranging from spin liquids to lattice-gauge theories. They appear to be particularly suitable for implementation of variational and quantum-classical algorithms, leading the search for first useful applications of quantum processors.

As described in the section "Long-Distance Quantum Communication and Applications of Distributed Entanglement," integrated quantum network nodes have been demonstrated recently using trapped cold atoms and ions, and color centers in diamond. In particular, quantum nodes combining all necessary ingredients—from efficient quantum-optical interfaces to long-lived memory and multiqubit operations—have been demonstrated recently using atom-like silicon vacancy centers in diamond. Proof-of-concept demonstration of emory-enhanced quantum communication has been carried out using system. These developments open up unique opportunities for realization of QRs for long-distance communication and for exploring new applications of quantum networks. In addition, these quantum networks provide a viable route for scaling up quantum processors to large-scale devices, by connecting small-scale quantum computers via quantum channels, thereby allowing quantum computation or simulation on quantum networks. It is one of the key features of atomic quantum hardware that quantum processors, involving local quantum memory and gate operations, representing the nodes of the quantum network, combine naturally with atom-photon quantum interfaces, enabling the needed conversion of "stationary" atomic to "flying" photonic qubits.

Recent advances demonstrating >20 dB spin squeezing, as well as in controlling coherent dynamics of strongly correlated systems, open the door for exciting applications of entangled states in quantum metrology. Exciting avenues range from the use of spin squeezing and entanglement to further improve the state-of-the-art optical atomic clocks, to realization of quantum sensor networks, and the use of strongly correlated states in systems ranging from ultracold atoms to solid-state atom-like systems to enable novel sensing functionalities and applications. Last, we expect that in the coming decade quantum sensors based on atom-like solid-state systems will be deployed for addressing long-standing goals such as single-molecule NMR and for realization of practical applications such as biomedical diagnostics and MRI on a chip.

Based on ideas from AMO physics, continuous-variable quantum information processing is making significant progress in the domain of microwave photons coupled to Josephson junction electrical circuit elements acting as artificial atoms. The first error-corrected logical qubit quantum memory to exceed the break-even point (i.e., achieve lifetime extension) for quantum error correction encoded the quantum information in a Schrödinger cat state of microwave photons (see the section "Cavity and Circuit QED"). A controlled-NOT entangling gate on two logically encoded photonic qubits was used for the first deterministic gate teleportation experiment. The one- and two-logical-qubit gate operations that have been developed for these cases are particular to the logical encoding used. The universal code agnostic entangling E-SWAP gate has recently been demonstrated for the first time and used to entangle two microwave cavities each holding a variety of different photon states. In addition, two superconducting qubits at opposite ends of a 78-cm microwave transmission line have been entangled with high fidelity. These advances represent substantial first steps toward construction of a modular architecture for quantum computation using error-corrected logical qubits that do not require vast overhead.

## FINDINGS AND RECOMMENDATIONS

**Finding:** There are many possible systems and platforms for construction of quantum machines. The technology development is still at a very early stage and the state of the art is evolving very rapidly.

**Finding:** The federal government has decided to pursue a "science first" policy for quantum information science.

**Recommendation: In support of the National Quantum Initiative, federal funding agencies should broadly support the basic research underlying quantum information science.**

**Recommendation: Academia and industry should work together to enable, support, and integrate cutting-edge basic research, complemented by focused engineering efforts for the most advanced quantum information science platforms.**

**Recommendation: The Department of Energy and other federal agencies should encourage medium-scale collaborations in quantum information science among academia, national laboratories, and industry.**

**Finding:** The Department of Defense has a long history of supporting AMO research as part of its mission. This has been richly rewarded by numerous developments including the laser, GPS, optics, and a multitude of sensors. More recently, the National Institute of Standards and Technology and the National Science Foundation have joined with the Department of Defense, leading to the emergence and nurturing of all aspects of QIS. Most recently, the Department of Energy is expected to play a major role in the National Quantum Initiative.

**Recommendation: (a) The Department of Defense (DoD) should continue both this foundational support for novel developments and the exploitation of the resulting technologies. (b) U.S. funding agencies participating in the National Quantum Initiative (NQI) should collaborate with each other and with DoD to build on the long history in quantum information science when developing their plans under NQI. (c) The Department of Energy and its laboratories should develop strong collaborations with leading academic institutions and other U.S. funding agencies to realize the full potential of quantum information science.**

# 5

# Harnessing Quantum Dynamics in the Time and Frequency Domains

When we watch a movie, we follow a plot and learn how a sequence of events unfolds in time. We also learn which interactions are important in driving events forward toward the end of the story. One of the fundamental goals of atomic, molecular, and optical (AMO) science is to assemble molecular movies of how electrons, atoms, and molecules interact with each other in real time, using ultrashort pulses of light or particles to take a series of "snapshots" that follow the dynamics. This will allow us to understand and subsequently control diverse processes such as how chemical reactions take place from the earliest stage to the end products; how the photoprotection mechanism in our DNA works to limit damage from ultraviolet radiation; or how a laser pulse can switch a current on and off in an insulator more than a trillion times per second. These dynamical processes take place on ultrafast time scales and are often exceedingly difficult to both measure and understand, since they generally involve strong correlations between different constituents, as well as transfer of energy among different degrees of freedom. The observation and control of such coupled dynamics thus require advanced investigative tools both experimental and theoretical.

For direct time domain access, the unprecedented development of ultrafast light sources as described in Chapter 2 has revolutionized the capabilities of AMO science to make molecular movies. This is illustrated in Figure 5.1, which shows how different types of dynamics take place on different characteristic time scales and are associated with different characteristic energies. For electrons, the natural time scale is tens to hundreds of attoseconds ($10^{-17}$ to $10^{-15}$ s), and this can routinely be accessed by attosecond pulses from high harmonic generation (HHG)-based,

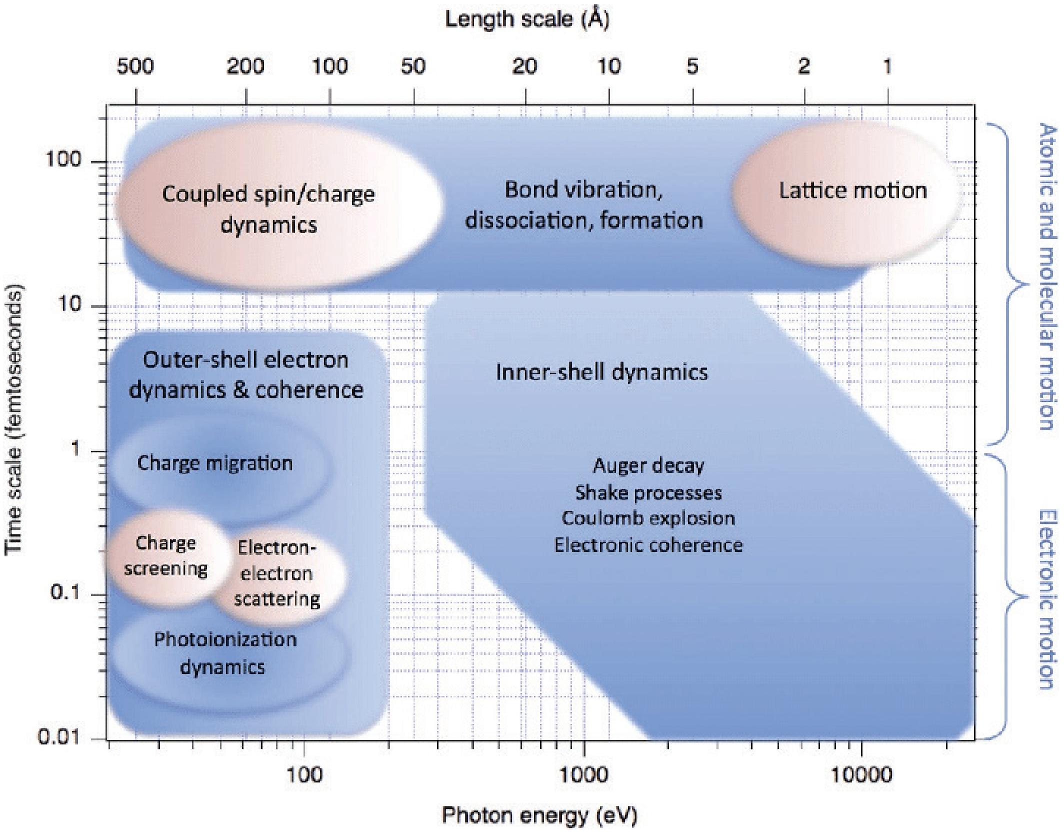

**FIGURE 5.1** This figure illustrates the time scales for different types of dynamics that can be probed with ultrafast sources, and the photon energies required to access them. Because they are so light, the dynamics of the electrons takes place on the fastest time scales (a few tens of attoseconds, $10^{-18}$ s), whereas the larger and heavier constituents such as atoms and molecules move on time scales of tens to hundreds of femtoseconds ($10^{-15}$ s). The figure also illustrates the characteristic energy scales for which these processes can be engaged. Inner-shell ionization that initiates electron dynamics, which in turn leads to chemical and structural dynamics, happens at photon energies of hundreds to thousands of electronvolts. The ionization from outer shells, leading to the fastest electron dynamics measured to date, can be done with soft X-ray light with photon energies below 100 eV. SOURCE: L. Young, K. Ueda, M. Gühr, P.H. Bucksbaum, M. Simon, S. Mukamel, N. Rohringer, et al., Roadmap of ultrafast x-ray atomic and molecular physics, *Journal of Physics B* 51:032003, 2018, https://doi.org/10.1088/1361-6455/aa9735, Creative Commons Attribution 3.0 license.

table-top sources of extreme ultraviolet (XUV) and soft X-ray radiation. The dynamics of the heavier nuclei takes place on time scales of tens to hundreds of femtoseconds ($10^{-14}$ to $10^{-12}$ s). The femtosecond pulses of hard X-ray radiation currently available from accelerator-based X-ray free-electron laser (XFEL) sources, with attosecond capabilities planned for the future, can access inner-shell electrons and probe the ensuing dynamics of the nuclei (termed molecular dynamics).

Because inner-shell transitions have energies that are characteristic of the local environment, these X-ray pulses allow scientists to focus on individual atoms even when embedded inside complex molecules. Another advantage of hard X-ray radiation is its very short wavelength, which is comparable to chemically relevant lengths scales, determined by bond-lengths of a few angstroms, and therefore allows for high spatial resolution when taking direct pictures of molecular structure via scattering of light. Ultrafast pulses of electrons have the same advantage, and recent developments have also allowed the making of molecular movies in which such electron pulses are taking the pictures. This chapter begins with a discussion on the making of molecular movies, starting with the attosecond electron dynamics and continuing with the femtosecond molecular dynamics.

Dynamical processes can also be accessed in the frequency domain, as evident from decades of knowledge gained from spectroscopy and collision physics. Although collisions are inherently time-dependent, collision physics often deals with phenomena at a fixed energy, and efforts by theory and experiment are devoted to understanding energy-dependent reaction rates. Such rates are frequently needed to model state-to-state collisional processes in gaseous environments, especially those with observable resonance phenomena. Collision theory, which connects with the observables of atomic and molecular spectroscopy, frequently involves solving the time-independent Schrödinger equation provided no time-dependent observation is carried out. Such theoretical descriptions are of interest when overall reaction rates for various processes are needed—for example, to describe how a gas cools in a terrestrial or atmospheric environment, or the chain of reactions that produces desired chemical reaction products. Even though the underlying phenomena may involve auto-ionization and other rapid electron transfer phenomena that occur in the femtosecond or attosecond time frame, such processes can still be treated within the framework of time-independent quantum calculations of the collisional dynamics. Collision experiments that measure such phenomena are highly sophisticated, and theory has made tremendous progress in its capability to describe increasingly complex reactions involving four or five atoms, but it is a challenge to push quantum theory capabilities to the point where it can handle systems with multiple complex reactants. This chapter also discusses dynamics accessed in the frequency domain, through collision physics theory and experiment, and through frequency comb spectroscopy.

Last, the committee discusses the novel physics that can be done with the extreme light sources of today. Chapter 2 described the extreme intensities that can be reached both in the optical regime, at pentawatt (PW) laser facilities, and in the X-ray regime, at XFEL facilities. The penultimate section of Chapter 5, "Novel Physics with Extreme Light," outlines some of the exciting science both within and beyond AMO that can be explored using such light sources. This chapter ends with a list of findings and recommendations.

## CHALLENGES AND OPPORTUNITIES

Direct experimental access to out-of-equilibrium dynamics and coupling between charges, spins, and atoms, together with their interpretation using advanced theoretical models, represents a grand challenge for both scientific and technological applications. Here, the committee outlines a number of exciting challenges and opportunities for the coming decade:

- Harnessing of coherent electron dynamics: Attosecond technology is enabling the measurement and control of electron dynamics in atomic, molecular, and condensed-phase systems. An exemplar is the concept of light-wave electronics in which a current in a semiconductor can be controlled with the electric field from a strong laser pulse, with potential for impact on the speed of electronic devices.
- Making of molecular movies, from electron to structural dynamics: The goal is tracking and controlling the flow of energy from electronic excitation through structural and chemical changes, spanning subfemtosecond to nanosecond time scales. This includes disentangling strong correlations between electrons, nuclei, and spins, with implications spanning the range from fundamental questions about energy transfer, to biological processes such as light harvesting, photoprotection, and to new molecular devices. In particular, recent advances in ultrafast X-ray sources, spectroscopy, and diffraction methods have us on the cusp of producing molecular movies starring individual molecules.
- Complex reaction dynamics and collision physics: The improvement of theoretical and experimental techniques that can predict reaction rates and unravel complex reaction dynamics of increasingly complex systems of atoms, molecules, ions, and photons is needed for deepening our understanding of chemical transformation processes and plasma environments.
- Extreme physics with extreme light sources: Light sources with extreme intensities, both in the infrared/optical regime and the X-ray regime, will allow for unprecedented studies of matter in extreme conditions with potential for numerous applications. X-ray strong-field physics, laser-assisted pair creation at the Schwinger limit, or laser-driven electron acceleration raise both fundamental questions and have significant potential for impact beyond AMO.

## ATTOSECOND SCIENCE: THE TIME SCALE OF THE ELECTRON

As discussed above, electrons in matter have very fast dynamics—on the time scale of tens to hundreds of attoseconds. Enormous progress in attosecond science and technology over the past decade means that researchers now routinely produce attosecond pulses and study attosecond processes using table-top laser facilities.

But what do we mean when we talk about "electron dynamics," since quantum mechanics teaches us that electrons should be described by their probability densities, which are distributed in space around the heavier nuclei in atoms and molecules? Electron dynamics in general means changes in the electron distribution following excitation. In the case of ionization, removal of an electron from an atom or molecule leads to a charge imbalance and therefore a rearrangement of the other electrons. Some examples of electron dynamics that can be measured and timed are photoemission (the absorption of a photon that leads to the release of an electron—how long does this take and which factors determine it?), ultrafast decay processes (for example, the filling of a hole after removing an electron from an inner shell), and charge migration (the coherent oscillatory motion of the electron cloud in a molecule resulting from the localized removal of an electron from a molecule). Some of these processes, and how to measure them, are described in more details below.

## Fundamental Questions on the Attosecond Time Scale

The photoelectric effect, which was first explained by Einstein more than 100 years ago, describes the emission of an electron following the absorption of a photon whose energy exceeds the system's binding energy. Starting in 2010, a series of experimental and theoretical works have explored the dynamics of the photoelectric effect. In the 2010 experiment, an attosecond XUV pulse freed electrons from two different orbitals in a neon atom (s and p orbitals) and their emission times were compared. The measurement showed a difference in the electron emission time from the two states ranging from 10-100 attoseconds. Continued progress in ultrafast laser development and metrology has allowed the accurate measurement of photoemission times in a range of systems, from atoms to semiconductors, as illustrated in Box 5.1. In the interaction between the ion core and the departing electron, the emission time can be interpreted in terms of the scattering phase imparted as the electron makes its way out from the ion core; this provides a concept of time in the quantum mechanical description of this process.

In a related set of experiments, the photoelectron emission resulting from strong-field ionization has been accurately timed using the so-called attoclock. In these measurements, the attosecond timing is provided by the rotating polarization of a near-circularly polarized laser field that tunnel-ionizes the atom. The polarization clock makes a full rotation every optical laser cycle, namely 2,700 as, and the electron will thus be emitted in different directions at different times during the cycle. In this way, attosecond dynamics are probed without the necessity of making an attosecond pulse.

Theory has played a crucial role in understanding the photoemission measurements. Fully quantum mechanical calculations of the dynamics of multiple

## BOX 5.1
## Timing the Photoelectric Effect in Metals

The photoelectric effect refers to the emission of electrons from a material following absorption of light. Progress in ultrafast metrology now allows researchers to measure the timing of this photoemission process, which happens on a time scale of a few to a few hundred attoseconds (as, 1 as = $10^{-18}$ s, or one billionth of a billionth of a second), depending on the material. Experiments rely on the precise timing of an attosecond extreme ultraviolet (XUV) pulse, which is absorbed and leads to photoemission, and an infrared reference pulse, which modulates the energy of the emitted photoelectron. By adjusting the delay between the XUV and the infrared pulse with attosecond precision, and studying the change in the photoelectron spectrum, one can measure the timing of the photoemission relative to a known reference. Figure 5.1.1 illustrates photoemission time measurements for electrons in a tungsten (W) sample. The most loosely bound electrons, in the W conduction band, exit the material in as little as 40 as. The researchers used both helium gas and iodine atoms as a reference in order to measure absolute photoionization times in W.

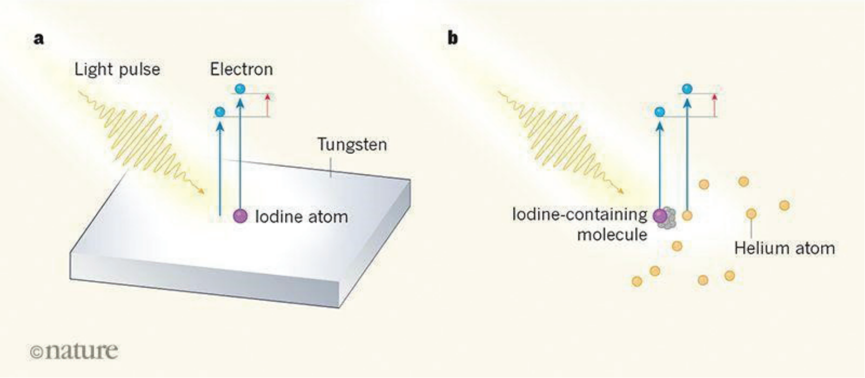

**FIGURE 5.1.1** Timing the photoelectric effect in metals. The absolute photoemission time from a tungsten surface is measured in a two-step process by relating it to photoemission times from other species: (a) An attosecond extreme ultraviolet (XUV) pulse (orange) leads to emission of electrons from the tungsten surface, as well as from iodine atoms deposited on the surface (blue arrows), and the authors measure the relative delay between the two electrons (red arrow). (b) Same as (a), but for electrons ejected from iodine-containing molecules and helium atoms in a gas. The absolute timing of the photoelectrons from the helium atoms can be calculated very accurately and used as a reference. SOURCE: Experiment by M. Ossiander, J. Riemensberger, S. Neppl, M. Mittermair, M. Schäffer, A. Duensing, M.S. Wagner, et al., Absolute timing of the photoelectric effect, *Nature* 561:374-377, 2018. Figure reprinted by permission from Springer Nature: T. Fennel, Timing the action of light on matter, *Nature* 561:314-315, 2018, doi:10.1038/d41586-018-06687-5, copyright 2018.

correlated electrons are possible only for small atomic systems, but these have allowed researchers to use measurements in helium as an absolute timing reference. Concepts gleaned from electron-ion scattering, well-known from collision physics, have been essential in the interpretation of these experiments, which are really measurements of the scattering phase, in terms of timing. Large-scale calculations of surface- and bulk-electron structure and dynamics have been necessary to understand emission times and laser interactions from condensed-phase materials.

Another fundamental ultrafast process is the decay that takes place in atoms, molecules, and solids. Molecules and most atoms have a range of core excited states that are inherently unstable. These have very short lifetimes, on the time scale of a few femtoseconds. Holes created in inner shells, for example, are often filled on this time scale by the decay of an electron in a higher-lying shell by emitting a photon (fluorescence) or another electron (Auger). This decay process can even happen between nearby atoms in a molecule or cluster so that an electron from one atom decays to a core hole in a neighboring atom. This process, called interatomic Coulombic decay, has recently attracted a lot of attention as it has been realized that it happens in a wide range of system and is important in some photobiological processes. As another example, coherent excitations from the valence band to the conduction band in insulators are thought to last only a few femtoseconds before they decohere by coupling to the crystal lattice degrees of freedom. These types of decay process can now be accessed in experiments combining ultrafast strong-field and attosecond methods.

Finally, charge migration is an important example of ultrafast coherent electron motion that occurs in a molecule following the rapid removal of an electron from either a core- or a valence shell to create a localized hole. This creates a charge imbalance in the molecule and can lead to the hole migrating across the molecule and back, on the time scale of one to a few femtoseconds, as has been reported by several groups for different molecules. Charge migration is strongly influenced by electron correlations, and is a precursor to more permanent charge- and structural rearrangements that happen over longer time scales. Calculations have suggested that there is in fact a universal attosecond response of many different molecules to a localized ionization event. Charge migration is an excellent exemplar for the earliest stages of a molecular movie, both in terms of the electron dynamics, which starts out coherent, and in terms of how the coherence is lost due to electron-nuclear coupling. Charge migration thus provides an exciting challenge for both experiment and theory in ultrafast AMO science.

### Intense Laser-Matter Interactions: A Gateway to Attosecond Science

In the first decade of the new millennium, the field of attosecond science was synonymous with the generation of attosecond light pulses in atomic gases via high harmonic generation. This is because the underlying physics of this generation process, based on an intense laser field (above $10^{14}$ W/cm$^2$) interacting with an atom or molecule, is inherently attosecond in nature. However, the attosecond light pulses are only one possible outcome of this strong-field interaction, and as illustrated above, attosecond science now drives a range of applications ranging from fundamental questions in quantum mechanics to filming molecular movies.

The physics of intense laser-matter interaction is well established by a plethora of experiments and theoretical analyses, which culminated in a widely accepted intuitive picture, the semiclassical recollision model. In this model, an atom or molecule subjected to an intense linearly polarized laser field is viewed in three steps, as illustrated in Figure 5.2. In the first step, an electron wave packet (EWP) is promoted to the continuum by tunnel ionization at some phase of the field. The wave packet then evolves under the combined influence of the field and atomic potential (step 2) until it either escapes or recollides with the parent ion after approximately one-half of an optical cycle (step 3). As illustrated in the figure, the recollision of the EWP with the parent ion leads to dipole emission, yielding high-energy photons (the high harmonics); the production of high-energy electrons; and sometimes multiple electron ionization. Most importantly, the initial tunnel ionization process, whose rate is exponential with the laser field, sets a time scale for the EWP that is inherently subcycle and therefore at the attosecond level. It is this EWP timing that is imprinted on all subsequent recollision processes.

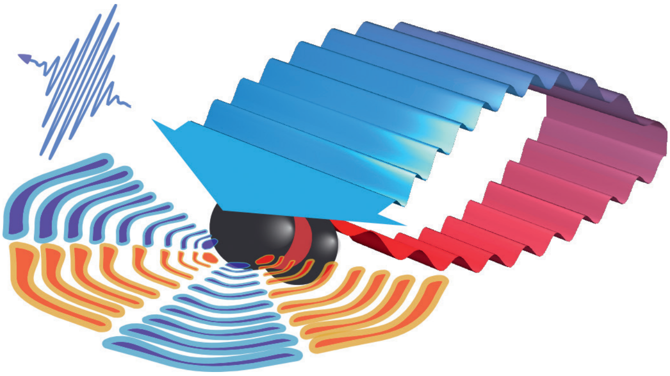

**FIGURE 5.2** An illustration of the semiclassical recollision model responsible for producing attosecond pulses and spatial-temporal molecular imaging. The essential physics is a field-driven electron wave packet (EWP) that self-probes the structure and dynamics of its parent ion upon recollision, through their shared coherence. The color-changing ribbon illustrates how the EWP is accelerated in the laser field so that it returns with kinetic energies of tens to hundreds of eV. In addition, the EWP is chirped during this interaction so that the high-energy part of the EWP returns to the core later than the low-energy part. This means that there is a simple relationship between time, on the attosecond time scale, and the energy of the emitted photons and electrons. SOURCE: See Laboratory Interactions, Dynamics and Lasers (LIDYL), "Strong-Field Rescattering Physics," http://iramis.cea.fr/LIDYL/Phocea/Vie_des_labos/Ast/ast_visu.php?id_ast=2881; courtesy of Stefan Haessler.

The three-step recollision model illustrates how the essence of strong-field attosecond science is the control of the EWP, which conveys additional ultrafast information via different observables. In high harmonic spectroscopy (HHS), as described in more detail below, the high harmonic light emerging from a molecule carries information about the molecular structure and dynamics in its spectral amplitude and phase. Figure 5.2 also illustrates another method for extracting molecular dynamics, termed laser-induced electron diffraction (LIED). This is the elastically scattered EWP—marked in the bottom left of the figure. The momentum distribution of the elastically scattered EWP process conveys information on the molecular structure, and LIED measurement provide a novel means for spatial-temporal imaging of molecular dynamics.

The recollision model has also been very influential in strong-field and ultrafast theory, through calculations based on the single-active-electron approximation, both at the ab initio and phenomenological level. In the past decade in particular, calculations based on the three-step recollision model, including quantitative calculations of the ionization probability, core and continuum dynamics, and complex rescattering cross-sections, have been used to interpret a number of experiments employing HHS and LIED to study atomic and molecular structure and dynamics.

From a fundamental perspective, harnessing the ultrafast and semiclassical nature of the EWP has been a major research thrust. AMO scientists have recognized that the scaling-laws of strong-field physics mean that experiments benefit from longer wavelength fundamental fields relative to the near infrared—for instance, leading to higher-energy photons and electrons while using lower intensity. The semiclassical three-step behavior described above has been firmly established using different laser platforms ranging from mid-infrared (1-5 microns) to terahertz generation. This strategy not only enables more applications but also has resulted in the discovery of new strong-field phenomena such as those described below.

## Strong-Field Attosecond Physics in Solids and Nanostructures

The insights of the recollision model are applicable not only to describing gas-phase processes, but also to the physics associated with a crystalline material interacting with an intense long-wavelength laser field. For example, nonlinear absorption across the bandgap in semiconductors and insulators generates emission through electron-hole recombination. Solids also provide additional processes absent in gas-phase systems. For example, a nonlinear current induced in a single band via Bloch oscillations generates harmonics. Studies have shown that both the recollision and the Bloch oscillation processes have a subcycle response (attoseconds) to the driving field. The interplay between these different mechanisms results in rich physics, and currently a variety of long- and short-range order in materials, including bulk and nanostructures, are under investigation. This is a very active area of research since it has the potential of providing a novel probe of band-structure dynamics, and perhaps the development of an on-chip vacuum ultraviolet (VUV) light source.

Nanostructures interacting with intense, few-cycle pulses also exhibit recollision model behavior, such as producing high-energy electrons and high-harmonic photons on very fast time scales as described above, with the physics of the dynamics again richer than in atoms. Exposing a metal nanotip to an intense field produces an electron energy distribution quite analogous to the well-known phenomenon of above-threshold ionization in atoms. Depending on the carrier envelope phase, electrons are emitted either from a single sub-500-attosecond burst or from two; the latter case leads to spectral interference. The interpretation is consistent with the coherent elastic scattering of a field-driven EWP. Unlike an atom or molecule, however, the nanotip produces a plasmonic enhancement of the local field, which decays rapidly from the tip. Thus, these experiments require only an unamplified ultrafast laser oscillator, since the intensities needed are orders of magnitude lower than the atomic case. Harnessing field-driven EWPs may provide new time-resolved methods for surface science. Low-energy electron diffraction, with electrons originating from and probing the surface yielding time scales of ~100 as, might come into reach.

### Attosecond Metrology: Methods for Clocking Electron Dynamics

The uncertainty principle says that one cannot simultaneously determine the precise energy and the precise timing of a physical process. As a result, an ultrashort attosecond pulse will in general excite a range of processes with different characteristic energies. To be able to resolve individual processes, attosecond metrology often relies on pump-and-probe experiments in which an ultrafast process is initiated with a pump pulse, and then probed by a second pulse that arrives some time later. The time resolution in the experiment is then determined by the precise control of the delay between the two pulses (which can be at the attosecond level), and the energy resolution is determined by the method of detection. By measuring how the absorption of an attosecond X-ray pulse changes as a function of this time delay (termed Attosecond Transient Absorption Spectroscopy, or ATAS), researchers have for example measured few-femtosecond lifetimes of states created by ionization or excitation, and specifically have observed the correlated motion of two quasi-bound electrons in helium, which "beats" with a periodicity of about 1 fs.

The standard picture of absorption is that of a quantum of energy being lost from the light field and stored in the material. However, in the time domain picture, absorption can be interpreted as the destructive interference between the electromagnetic field of the input light and the light resulting from a coherent oscillation created in the material. This means that the absorption process can be interrupted and controlled by a probe infrared laser field. In the spectral domain, this manifests as a change of the basic shape of the absorption peak in the X-ray spectrum, and has wide-ranging consequences for potential control of the temporal and spatial properties of X-ray pulses. Absorption along one direction can, for example, be refashioned as emission along a different direction, leading to the modulation of X-ray light by an optical field.

In HHS, the time resolution is provided by the time-frequency ordering of the returning EWP in the semiclassical recollision model: the electrons that give rise to the higher photon energies return later than the low-energy ones. This means that different frequencies in the harmonic spectrum carry information about different recollision times, at the sub-laser-cycle (and thus attosecond) time scale, and the resulting chirp of the emitted harmonic radiation has been dubbed the attochirp. HHS has been used in a wide range of applications, measuring atomic and molecular structure and dynamics, both at the electronic (charge migration) and nuclear (dissociation) level, and more recently to characterize both structural and dynamical features in solids.

There are also several attosecond clocking methods based on measuring photoelectrons, in particular measuring their spectral yield as a function of a time delay that is known with attosecond precision. This is the basis for attosecond streaking and RABBITT (both discussed in Chapter 2) and the attoclock. The timing of the photoelectric effect (see Box 5.1) was performed using the attosecond streaking method. Lastly, the ability to control and measure the polarization properties of high-order harmonics has exciting implications for the characterization of spin, magnetic, and chiral properties and dynamics of gas- and condensed-phase samples. This polarization control, which has been demonstrated and explored in detail in this past decade, is achieved by generating harmonics with counter-rotating two-color laser fields, leading to harmonic radiation with any choice of linear, elliptical, or circular polarization. The chiral properties of a sample can then be probed either through the imprint of the sample on the harmonic properties (similar to HHS), or by examining the response of the sample subjected to polarized XUV or X-ray light.

## Challenges for Theory

Calculating attosecond electron dynamics from first principles in molecular systems, like biomolecules, is one of the premier computational challenges today and will remain so for the foreseeable future. The fundamental difficulty is the rapid scaling of the computational effort with the number of active electrons. This is particularly true because most attosecond dynamics involves ionization, which necessitates being able to describe multielectron continuum as well as bound states. Progress in the past decade has allowed a number of fully ab initio studies of correlated electron dynamics in helium and other two-electron systems, treating strong-field double-ionization, two-XUV-photon ionization, and questions of photoionization timing as discussed above. Efforts are underway to gather a number of these highly validated theoretical approaches in a common Atomic and Molecular Physics Gateway, which will include access to software suites and documentation for other research groups. Calculations in larger systems can in principle be attacked by including multiple, time-dependent configuration interactions. This has been done for small systems using configurations including single and double excitations, and it is an active area of research to extend such approaches to more complex and/or nonlinear systems. An alternative, approximate treatment using time-dependent density functional theory (TDDFT) has the attractive feature that it can be scaled to large systems. TDDFT has been shown to be accurate enough for single ionization and charge migration studies, but also raises open questions about how to calculate certain observables from the density, as well as its reliability to describe processes with correlations beyond the mean-field level.

The next-level problem in calculating coherent electron dynamics will be to include the coupling to the inevitable nuclear dynamics and the ensuing loss of electronic coherence. For molecules, only hydrogen-like systems with two nuclei and two electrons have been treated fully ab initio, for example for studies of electron localization upon strong-field ionization, or the influence on nuclear dynamics on transient absorption spectra. Calculations of ultrafast electron dynamics in condensed-phase systems have been undertaken by a number of groups in the past few years, as experimental interest has flourished as described above. Most of these have been done in periodic, crystalline systems in which many-body interactions can be managably treated, for instance using the semi-conductor Bloch equations. However, also for these systems, the loss of electronic coherence via for instance coupling to the nuclear degrees of freedom has generally been treated phenomenologically. Much work still needs to be done, for both molecular and condensed-phase systems.

### The Future of Attosecond Science

Attosecond science is beginning to impact our understanding in condensed-phase systems, with implications for both XUV source development and ultrafast metrology. For example, progress on the implementation and understanding of HHG in solids suggests that compact and efficiently engineered sources of ultrafast XUV light are feasible. The use of pump-probe methods to determine attosecond photoemission times from metals, and attosecond lifetimes of conduction band electrons in semiconductors, means that attosecond metrology is capable of probing the fastest dynamics even in such highly correlated systems.

The concept of lightwave electronics is particularly exciting. The increase in speed of modern electronics is a consequence of shrinking electronic devices. However, the sizes are rapidly approaching the ultimate nanoscale limit; thus, the clock rate (processing speed) has been limited to a few gigahertz for more than

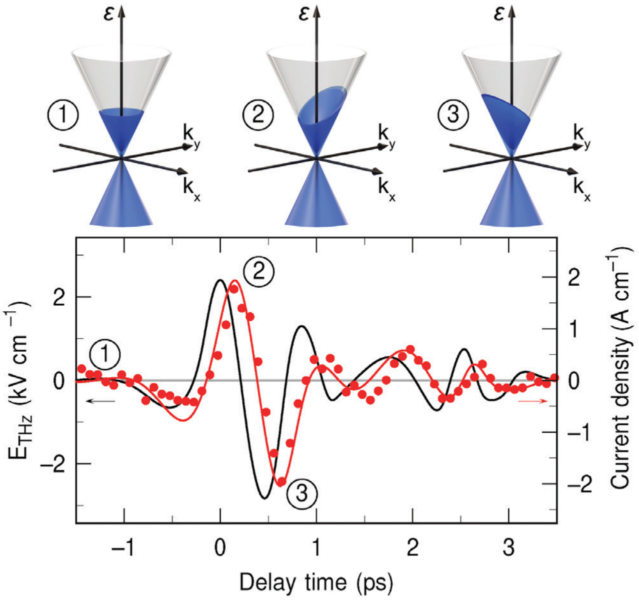

**FIGURE 5.3** This figure illustrates the prospect for lightwave electronics. The Dirac cones at the top illustrate the electron momentum distribution in the topological insulator bismuth telluride, at three different delay times as the electrons are being accelerated by an intense terahertz light field. The graph below illustrates how the resulting electric current (as measured by the red data points) is driven by the direction of the terahertz electric field (black line) at a clock rate corresponding to that of the laser frequency. SOURCE: Experiment by J. Reimann, S. Schlauderer, C.P. Schmid, F. Langer, S. Baierl, K.A. Kokh, O.E. Tereshchenko, A. Kimura, C. Lange, J. Güdde, U. Höfer, and R. Huber, Subcycle observation of lightwave-driven Dirac currents in a topological surface band, *Nature* 562:396-400, 2018; courtesy of U. Höfer, Marburg University.

a decade. Recent experiments have demonstrated lightwave control of electronic currents in insulators, in which a strong laser field induces and modulates a time-dependent electric current in the material (see Figure 5.3). These laser-induced currents are generally reversible and nearly dissipation-free. Given that strong laser fields can be produced with optical periods close to the petahertz level, this suggests that lightwave-driven currents in transistors could result in speed-up of many orders of magnitude in the near future.

Another exciting prospects for attosecond science is the impending availability of intense attosecond pulses in the soft and hard X-ray regime from XFELs, which would enable the initiation of electron dynamics (e.g., charge migration) from inner valence or core electrons that are in general highly localized on specific atoms within a molecule. In combination with pump-and-probe capabilities, such pulses would thus allow for both spatial and temporal resolution of attosecond electron dynamics.

## THE MOLECULAR TIME SCALE: FEMTO- TO PICOSECONDS

At the heart of any chemical reaction is explosive transformation: old bonds in a molecule are broken and new ones formed. In photochemistry, rapid ionization of a system leads to rapid electron motion, which leads to atomic displacements, which leads to chemical changes. Light harvesting in chromophores, the photoprotection mechanism in our DNA, and more generally optically driven molecular devices are all examples of processes in which an initial electronic excitation is coupled to nuclear motion that leads to chemical or structural changes. In the previous section, the committee discussed that the initial electron motion takes places on sub-to-few femtosecond time scales and often involves electron-electron correlation. This section focuses on primarily the subsequent molecular dynamics that happens over tens to thousands of femtoseconds and involves both electron-nuclear and nuclear-nuclear correlations.

### Molecular Dynamics and the Concept of Femtosecond Molecular Movies

The nuclear dynamics discussed above includes both motion, such as vibrations, rotations, and structural/configurational changes of the molecule, and changes in the charge-, spin-, or oxidation state. Electrons always play a role in the nuclear dynamics, since the molecule will always seek to be in the configuration with the lowest electronic energy. The interaction between the electronic and nuclear degrees of freedom can often be thought of in the Born-Oppenheimer approximation, in which the electron and nuclear dynamics are treated separately (based on the different time scales for their dynamics) so that the electronic density simply creates the potential surfaces on which the nuclei move. However, there are also many interesting instances in which the electronic and nuclear dynamics is much more directly coupled, so that the Born-Oppenheimer approximation breaks down. This is often seen in the form of conical intersections (CIs)—where different molecular geometries give rise to electronically excited states with the same energies. At such points, an electronic excitation in one nuclear configuration can therefore result in population transfer to a different nuclear configuration, thereby driving structural changes in the molecule. These CIs, spanning the space between the physics of coherent electron dynamics and the chemistry of transformation, have been topics of intense interest in the ultrafast AMO community, and have been documented both in naturally occurring transformations as well as controlled by ultrafast light pulses.

Ultrafast pulses of light or electrons are ideal tools to see the nuclear motion directly in the time domain, as first demonstrated by one of the the founders of “femtochemistry,” Ahmed Zewail, for which he was awarded the 1999 Nobel Prize in Chemistry. An example of such a femtosecond molecular movie is illustrated in Box 5.2. The individual pictures in the movie can consist of any measurement

## BOX 5.2
## X-Ray Movies

Movies are made by putting together still pictures taken at different times during an evolving process. To avoid blurring, each picture must be taken during such a short time that the process appears frozen. Figure 5.2.1 illustrates how to make a molecular movie of a light-induced structural transformation, in which the original ring-shaped structure of gas-phase molecules is opened to a chain-shape within 100 fs after the initial excitation. The ultrafast X-ray pulses from the Linac Coherent Light Source (LCLS) are so short and so bright that the diffraction pattern samples the molecular structure at a particular time after excitation. Calculations show that this electron-assisted structural change happens through a conical intersection, and that it involves a reshuffling of electron bonds: In the ring-shaped molecule there are double-bonds between two of the carbon sites, whereas in the chain-shaped molecule there are three double-bonds.

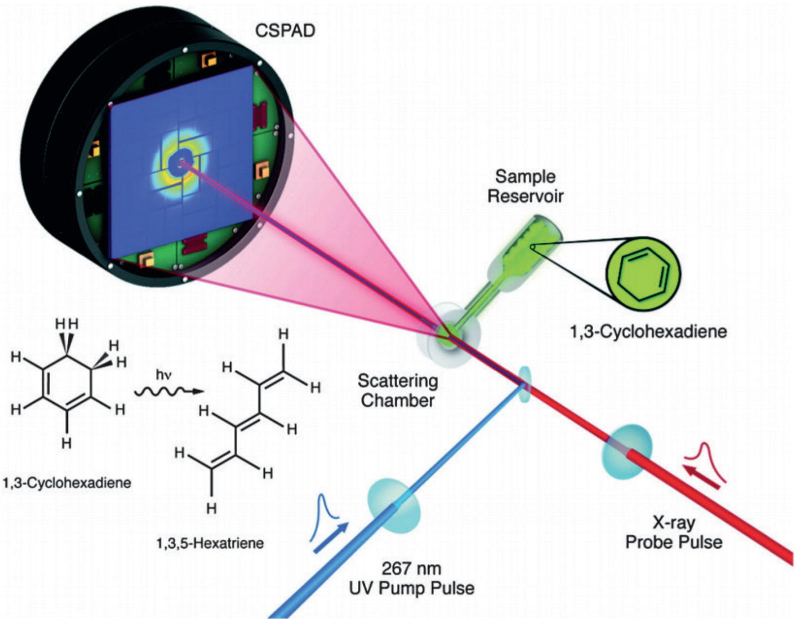

**FIGURE 5.2.1** X-ray movies of molecular dynamics. A pump UV pulse (blue) initiates the ring-opening reaction, and the scattering pattern from a delayed X-ray probe pulse (red) is recorded on the detector (CSPAD) as a function of time delay between the pump and the probe pulse. This allows researchers to "film" how the molecules change shape after the excitation, from an original ring-shape to a final chain-shape. SOURCE: Reprinted figure with permission from M.P. Minitti, J.M. Budarz, A. Kirrander, J.S. Robinson, D. Ratner, T.J. Lane, D. Zhu, et al., Imaging molecular motion: Femtosecond X-ray scattering of an electrocyclic chemical reaction, *Physical Review Letters* 114:255501, 2015, https://doi.org/10.1103/PhysRevLett.114.255501; copyright 2015 by the American Physical Society.

that is sensitive to the instantaneous electronic or structural configuration of the molecule, and it can be direct in the form of actual images such as scattering patterns, or indirect in the form of absorption or emission spectra, or the detection of ions or photoelectrons. Several of these approaches are discussed in more detail in the subsections below.

The access to and control of ultrafast light pulses, ranging from the optical through the hard X-ray spectral range, continues to drive immense progress in time-resolving fundamental processes in molecules and beyond. An exemplar for advances in ultrafast technology in the past decade, as well as an illustration of coupled electron-nuclear dynamics driving a configurational change, is the photo-induced ring-opening reaction in 1,3-cyclohexadiene. This well-known photobiological reaction plays a role in vitamin D synthesis, and involves an opening of the initial ring-shaped molecule to the final chain-shaped 1,3,5-hexatriene molecule, which takes place on the 100 fs time scale. The ring-opening reaction involves a reshuffling of single and double electronic bonds, and proceeds through a conical intersection. Progress in ultrafast metrology has allowed this reaction to be probed directly in the time domain, in three different types of experiments in the past decade: (1) hard X-ray diffraction as illustrated in Box 5.2; (2) soft X-ray absorption spectroscopy; and (3) ultrafast electron diffraction, both of which are discussed in the sections below.

## The Ubiquity of Ultrafast X-Rays

The unprecedented development of ultrafast XUV and X-ray sources in the past decade, both XFEL sources and XUV table-top sources based on HHG as described in Chapter 2, has revolutionized the capabilities of AMO science to probe ultrafast dynamics. The short duration and high photon energies of these modern X-ray sources enable scientists to focus on individual atoms, even when embedded in complex molecules, and to view electronic and nuclear motion on their intrinsic time and space scales.

Soft and hard X-ray pulses generally probe different aspects of the electronic and nuclear dynamics, and different types of experiments can therefore elucidate the connection between the initial electronic dynamics and the subsequent molecular dynamics in a molecule that has been excited by an optical or X-ray pump pulse. As also discussed in the section "Attosecond Science: The Time Scale of the Electron," soft X-ray and XUV pulses address the structure and dynamics of valence electrons with their moderate binding energies, whereas hard X-ray pulses with their very short wavelengths can be used to resolve the location of nuclei directly through scattering images, as was illustrated in Box 5.2.

These experiments also benefit from the extension of well-known X-ray spectroscopy techniques into the femtosecond domain, and from an unprecedented degree of control over the initial preparation of the sample, the relative timing of the pump and probe pulses, and the extraction of information from the detection step. In sample preparation, in particular, the ability to align and orient gas-phase molecules using lasers means that the molecular dynamics can often be explored in three dimensions, as the ion and photoelectron yield can be measured as a function of the relative orientation of the molecule and the polarization of the light field. Several methods allow for detection of all or several dynamics constituents in coincidence, vastly increasing the amount of information gained about how the dynamics proceeded. Among these are velocity map imaging and Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS).

X-ray absorption and photoemission spectroscopy can also be used to infer molecular dynamics via the measurement of characteristic electronic transitions, especially between core- and valence-level states. This is because the electronic excitations energies are characteristic of the nuclear configuration, including its charge-, oxidation, and spin-state. This is the basis for time-resolved X-ray absorption spectroscopy "movies," an example of which is illustrated in Figure 5.4 for the dissociation of tetrafluoromethane. In this molecule, the increase in the

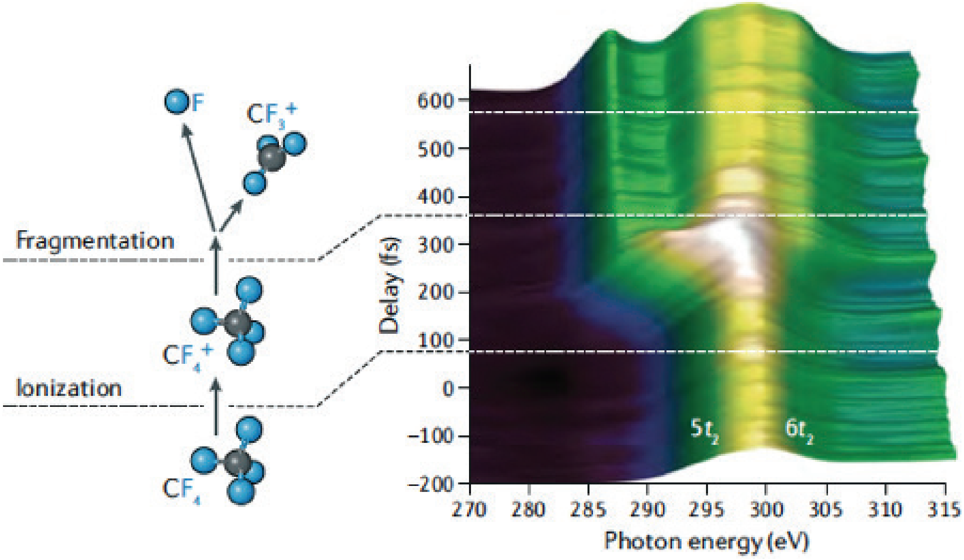

**FIGURE 5.4** The left side of the figure shows schematically how the molecule tetrafluoromethane ($CF_4$) breaks apart after an electron is removed from it. The right side illustrates how this fragmentation can be followed via time-resolved X-ray absorption spectroscopy. The characteristic X-ray absorption energy is sensitive to the length of the C-F bond, so that a new absorption peak appears and changes energy as the delay between the initial ionization laser pulse and the probe X-ray pulse is changed. SOURCE: Adapted from Kraus et al., *Nature Reviews Chemistry* 2:80, 2018.

internuclear separation between the F atom and the remaining $CF_3^+$ group gives rise to a characteristic new peak in the core-level absorption spectrum.

Time-resolved soft X-ray absorption spectroscopy was also used to investigate the ring-opening of cyclohexadiene. By following the evolution of characteristic core-to-valence transitions with delay, AMO scientists were able to directly reveal the intermediate (transient) electronic state that the ring-opening reaction proceeds through, the so-called pericyclic minimum. This represents information complementary to the purely structural information about the location of the nuclei during the reaction, helping to shed light on the coupling of the electronic and nuclear degrees of freedom.

The characterization of electrons or ionized fragments resulting after X-ray ionization or excitation of deeply bound states can also elucidate the interaction between the electronic and molecular dynamics. Electronic kinetic energies, for example, whether from direct photoelectrons or Auger electrons, are sensitive both to particular bond lengths (as also discussed above) near the atomic site from which they originated, and to the electronic states involved in the photochemical reaction. In a recent example, researchers were able to solve a long-standing controversy involving the photoprotection mechanism of the DNA-compound thymine. By combining Auger electron and soft X-ray absorption spectroscopy, and via comparisons with theory, they found that after UV photoexcitation, the molecule relaxes into the protected (less chemically reactive) state via a conical intersection in less than 100 fs.

Hard X-ray radiation is ideal for taking direct pictures of molecular structure through scattering images, because their short wavelengths, comparable to common bond lengths, permit very high spatial resolution. Hard X-ray radiation was used in the direct imaging of the ring-opening reaction illustrated in Box 5.2. This type of imaging through diffraction, using ultrafast pulses of light or electrons, is discussed in the following section.

## Molecular Imaging Through Ultrafast Diffraction

A multitude of diffraction techniques exist to take "pictures" of molecular samples during a dynamical process, and more broadly to image the structure of noncrystalline samples at the atomic level. The scattering pattern on the detector is not in general a straightforward image of the sample (like that formed by a camera) but has to be interpreted using sophisticated Fourier-transform-based algorithms. Coherent diffractive imaging (CDI), for example, takes advantage of the high spatial coherence of the laser-like ultrafast X-ray pulses from HHG and XFEL sources to retrieve both amplitude and phase information from the diffraction pattern, leading to increased sensitivity and contrast. For imaging of gas-phase ensembles, the phase can often be retrieved directly from the Fourier transform of the scattered data. For more complex (e.g., crystalline) samples, the phase retrieval is based on hundreds or thousands of iterations of an algorithm that goes back and forth between the measured diffraction pattern on the detector and the real-space image of the sample. In each iteration, more constraints can be applied since the high quality of the X-ray beam allows for oversampling of the spatial structure of the sample. By controlling the polarization of the X-ray light, or in combination with its X-ray absorption spectroscopy, CDI enables mapping of the elemental, chemical, and magnetic properties of complex matter at the nanoscale.

Single-particle imaging (SPI) has long been a dream of several communities, both as an element of making molecular movies, but more generally for imaging in structural biology and materials science. Inroads are now being made toward this goal, thanks to the advent of the very intense and short pulses of X-ray light available at XFEL facilities. Imaging a single biomolecule presents a number of technical and computational challenges. First, the scattering from a single molecule is very weak, and even when using intense X-ray sources, the scattering pattern from many different individual molecules, generally with different orientations, must be analyzed using CDI techniques discussed above, and added together to give three-dimensional (3D) information. Second, the intense X-ray light causes the molecules to explode. However, if the pulse is short enough, then the scattering pattern can be formed before the damage occurs. A global SPI initiative, launched in 2014 and drawing on significant multidisciplinary effort from research groups around the world, has been devoted to resolving current and future challenges in SPI. In 2015, researchers presented the first 3D measurements of a single biological sample, the large 750-nm-diameter mimivirus, with a spatial resolution of 125 nm. More recently, several smaller viruses have been imaged with spatial resolutions below 10 nm, as illustrated in Figure 5.5.

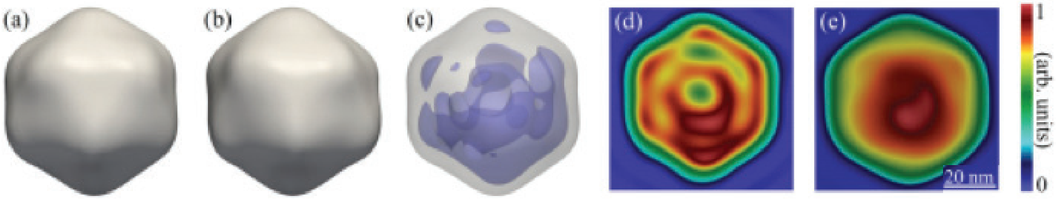

**FIGURE 5.5** Mapping of rice dwarf viruses, reconstructed from several million X-ray diffraction images of individual virus molecules. Two different views of the outside of the virus are shown in (a) and (b). (c) to (e) show the nonuniformity of the internal distribution of material inside the virus, in the form of a density plot in (c) and in two-dimensional slices in (d-e). SOURCE: Reprinted figure with permission from R.P. Kurta, J.J. Donatelli, C.H. Yoon, P. Berntsen, J. Bielecki, B.J. Daurer, H. DeMirci, et al., Correlations in scattered X-ray laser pulses reveal nanoscale structural features of viruses, *Physics Review Letters* 119:158102, 2017, https://doi.org/10.1103/PhysRevLett.119.158102; copyright 2017 by the American Physical Society.

Ultrafast electron diffraction (UED) is a complement to ultrafast X-ray diffraction; it benefits from larger electron scattering cross-sections. Advances in the production and stability of femtosecond pulses of high-energy electrons have allowed a number of studies of dynamics using an optical pump and a UED probe. Recent examples include mapping the ultrafast photo-induced dissociation dynamics of $CF_3I$ molecules in the gas phase via a conical intersection that allows the transfer of the initial electronic excitation energy to the nuclear degrees of freedom responsible for the dissociation. In another recent study, the very high spatial resolution provided by the electron beam allowed researchers to follow the evolution of individual carbon-carbon bonds during the ring-opening reaction in cyclohexadiene (also studied in the X-ray scattering experiment in Box 5.2), yielding not only a detailed movie of the ring opening itself but also evidence that the chain-shaped molecule after opening bends back and forth between two different configurations.

In LIED, the ultrafast electron "pulse" is generated by a strong laser field as the rescattering EWP discussed in the context of the three-step model for intense laser-matter interactions above (see Figure 5.2). This self-probing of a system set in motion by strong-field ionization has proven to have high resolution in both space and time, with recent measurements of the ultrafast dissociation of acetylene, for example, or the laser-induced structural deformation of the $C_{60}$ cage.

## Using Light to Control Reaction Paths

Light can be used not only to initiate and probe a dynamical process but also to control how the process unfolds. This is generally referred to as *quantum control.* The past decade has continued to see extensive developments. There are several different approaches to quantum control including ones that exploit optical lattices in reduced dimensionality, and ones that exploit excitation to and from, and dynamics on, different potential energy surfaces, designing system-specific pump-probe sequences. Some methods have their own names, like *optimal control* and *coherent control*, respectively.

The optimal control approach relies on the ability to control a range of parameters influencing the shape of an ultrafast light pulse that interacts with the system of interest so that a desired outcome can be achieved, often using a feedback loop and some number of iterations. Early experiments used precise shaping of the driving laser pulse to control ionization, dissociation, or emission properties in small quantum systems, as well as reaction pathways in chemical reactions, for example, via light-induced conical intersections. For current and future studies, the continued progress in machine learning and big-data analysis enables the control of a much larger range of laser and environmental parameters, potentially making outcomes more robust and repeatable.

The coherent control approach involves building creative control scenarios by harnessing the underlying quantum mechanics—for example, exploiting interferences between different pathways to the same final product state to control, for example, product branching ratios, photoassociation, enantiomeric selectivity, state-to-state control, and spin-orbit entanglement in atom pairs. Other recent applications include biexciton control in quantum dots, pulse train control, and producing chains of entangled ion-atom pairs. It also has opened a view into foundational issues such as examinations of the role of "nontrivial" quantum effects (such as interference, nonlocality, and entanglement) in control scenarios, considerations of classical limits on control, and recognition of the role of *in-principle* distinguishable pathways in diminishing control. Important challenges remain in the area of understanding and controlling decoherence.

### Quantum Calculations of Molecular Dynamics

Predicting the nuclear motion and structural dynamics for hundreds of femtoseconds after some initial excitation requires the description of both electronic processes, such as excitation and charge transfer, and nuclear dynamics facilitated by transitions between electronic states. Even without taking into account electronic coherence, this is a grand-challenge-level computational problem, and major efforts are dedicated to its solution.

One such theory approach, termed ab initio nonadiabatic molecular dynamics, uses methods from quantum chemistry to solve the time-independent electronic Schrödinger equation to obtain electronic structure, simultaneously with quantum descriptions of the nuclear motion and transitions between electronic states. Recent progress has allowed a number of high-level comparisons to experimental results, showing very good quantitative agreement with theoretical predictions—for example, for both of the UED experiments described above, on the ring-opening reaction and the dissociation of $CF_3I$. A key bottleneck for going forward is the molecular size and degree of correlations that can be modeled with such approaches, due to both scaling with system size issues and the vastly different time scales that need to be computed for the electronic and nuclear motions. Improvements in the treatment of quantum effects in the nuclear dynamics and the solution of the electronic structure problem for large molecules are both critical to further progress. In order to even qualitatively model conical intersections, where multiple electronic states are degenerate, multireference electronic structure methods are needed. At the same time, dynamic electron correlation effects can be important in changing the location and energetics of conical intersections. Thus, both static and dynamic electron correlation effects must be included. In order to simulate and understand charge and energy transport in large-scale molecular assemblies (relevant in application areas such as artificial photosynthesis and batteries), it is therefore critical to improve methods for incorporating static and dynamic electron correlation simultaneously with nuclear motion.

New conceptual approaches to these problems are critical, but it is also important that they be adapted to and implemented on fast and efficient computer architectures. The emergence of graphical processing units (GPUs) as computational engines for physics and chemistry, has highlighted the importance of "stream processing"—that is, extreme data parallelism—as well as exploitation of heterogeneous architectures such as combinations of CPUs and GPUs. Some of the algorithms for electronic structure theory and molecular dynamics have been recast in a form suitable for efficient execution on these architectures, which will almost certainly play a key role in the path to exascale computing. Much more effort along these lines is needed, especially in a manner that creates building blocks that are easily reused and retooled so that they remain relevant when new conceptual approaches appear.

### The Role of Quantum Chemistry in Spectroscopy and Dynamics

The calculation of molecular energy spectra, for both ground-state and excited-state molecules, is the basis for comparison with and predictions for a wide range of experiments in high-precision or time-resolved spectroscopy. A number of large-scale packages for quantum chemistry calculations exist, and are continuously being developed and applied. The need to treat molecules with a large number of quantum constituents, and with highly correlated electrons, drives developments in quantum chemistry, including both improvements in precision and in the scaling of resources with the number of electrons. Recent notable developments include advances in various forms of quantum Monte Carlo (QMC) as well as the development of methods in density-matrix renormalization group (DMRG) better able to deal with quantum chemistry. While QMC methods have been considered the gold standard for accuracy for several decades, they have until recently been computationally costly. In the past decade, advances in the initial trial wave functions used in QMC have allowed both improvements in precision and computational scaling for a range of moderately sized systems. Similarly, DMRG methods have been gaining attention in the quantum chemistry community recently, also for their potential to both increase precision and computational efficiency. A recent example of the latter includes studies of long chain molecules for which the computational time scales linearly with chain length.

### The Future of Time-Resolved Molecular Dynamics

Modern ultrafast X-ray sources provide shorter pulses, a wider selection of photon energies, and higher brilliance than ever before, and will in general enable better resolved dynamics in both space and time. For example, the increased brightness that will soon be available at the upgraded LCLS facility (LCLS-II) makes it very likely that the next decade will see time-resolved dynamics at the single-particle level. Similarly, the impending availability of X-ray pump, X-ray probe capabilities, using intense pulses for which the photon energy and the relative delay can be controlled, will enable nonlinear spectroscopy studies that involve multiphoton transitions. Nonlinear spectroscopy—for example, Coherent Anti-Stokes Raman Scattering—using a carefully timed series of optical pulses, has long been a favorite tool for studying electron and molecular dynamics, and its extension to the X-ray regime is an active area of research. Its extension to the X-ray regime would allow making "complete" molecular movies spanning both spatially resolved, attosecond, core, and valence electron dynamics, as well as couplings to femtosecond nuclear dynamics. For instance, one could track the ultrafast passage through a conical intersection and its impact on electronic coherence. Additionally, ultrafast AMO science will have far-reaching consequences for applications to photobiology. Figure 5.6 shows an example of the photo-induced dynamics in the retinal-binding protein bacteriorhodopsin. Retinal is a light-sensitive molecule

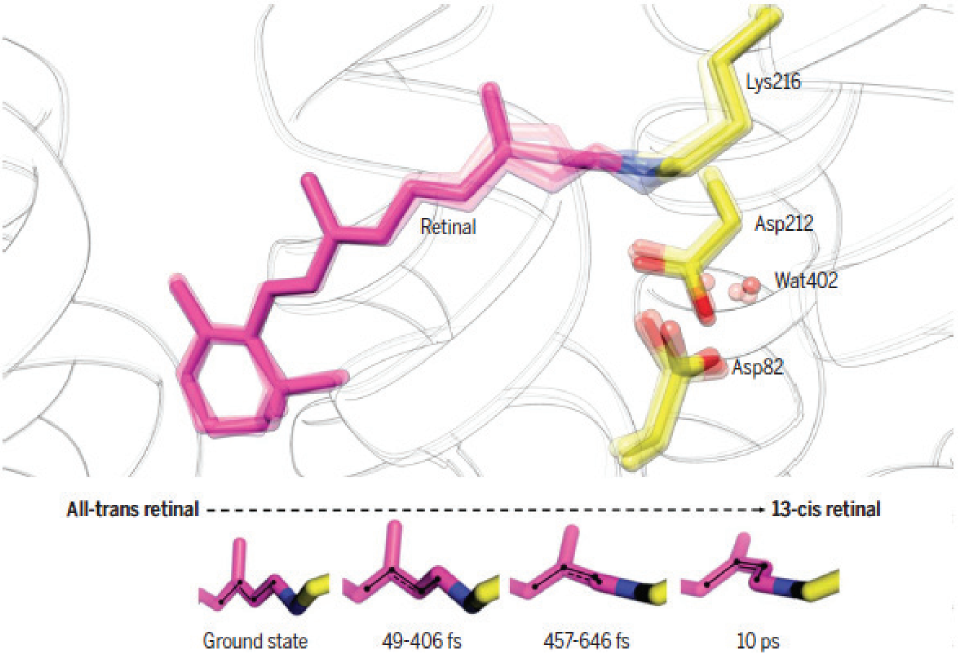

**FIGURE 5.6** The structural rearrangement of the light-harvesting protein-ligand retinal, following photoexcitation, was captured using time-resolved ultrafast X-ray crystallography. The evolution of retinal and the surrounding protein happens over a few hundred femtoseconds, in response to changes in electronic structure induced by photoabsorption. Informed by large-scale molecular dynamics calculations, scientists were able to interpret the dynamics in terms of breakage and formation of individual bonds. SOURCE: From Nogly et al., *Science* 361, 145, 2018.

that is used biologically in a range of light-harvesting and light-energy transfer processes, and its structural rearrangement (isomerization) takes place in tens to hundreds of femtoseconds, making it among the fastest known in photobiology. Researchers captured its transformation in real time using time-resolved ultrafast X-ray scattering.

Last, optical pump and X-ray probe studies will enable a wide range of studies of new phases of matter, including quantum materials, induced by coherent light-matter couplings. Recent exciting examples include the demonstration of light-induced superconductivity, and control of topological phases via the polarization of the excitation light source. A theoretical prediction for the ability to switch a material between a topological insulator and a conducting semi-metal using femtosecond laser sources could potentially be experimentally validated using diffraction of hard X-ray pulses from soon-to-be-available XFEL sources.

## FREQUENCY-DOMAIN APPROACHES TO DYNAMICS: COLLISIONS AND CORRELATIONS

The sections above have discussed how the increased temporal resolution provided by femtosecond laser sources enables the study of ultrafast dynamics directly in the time domain. Likewise, the unprecedented spectral resolution provided by phase-controlled continuous wave lasers enables the study of ever finer energy structures of matter. For example, it is now possible to investigate optical transitions with a resolution approaching 1 part in $10^{16}$. Many new scientific thrusts have emerged through this quest, such as tests of fundamental physics, the development of sensors of increasing sensitivity, and the search for new physics beyond the standard model.

For much of the past half-century, efforts by theory and experiment were mostly devoted to understanding energy-dependent reaction rates, in contrast to the recent emphasis on time-dependent processes that has been enabled by the advent of ultrafast lasers and detection techniques. Complementary to time-resolved experiments, the energy-resolved results from collision studies is what is frequently needed to model state-to-state collisional processes in gaseous environments, especially those with observable resonance phenomena. Advances in both time- and frequency-domain approaches are still needed, in order to achieve deep understanding and accurate predictive power of quantum mechanical processes, especially at low collisional energies or temperatures. In particular, significant fundamental progress is needed to extend current theoretical capabilities to quantitatively treat and unravel collision events involving four or more atoms or small molecules.

It should also be stressed that the possibilities are not restricted to “time-only” resolution or “frequency-only” resolution. In some cases, it is desirable to obtain both time and frequency resolution of dynamical processes simultaneously, and this is possible within the usual constraints imposed by the frequency-time uncertainty principle.

## Frequency Combs—A New Frontier in Broadband and High-Precision Spectroscopy

Optical frequency combs offer enormous potential owing to the simultaneous availability of vast spectral coverage and high spectral resolution, and they open a new frontier for coherent spectroscopy and broad-bandwidth, high-resolution quantum control of molecular dynamics. As discussed in Chapter 2, these combs emerge when phase stabilization is applied to a periodic train of femtosecond mode-locked laser pulses, yielding control over both the repetition frequency and the optical carrier with respect to the pulse envelope. The broad spectral coverage of the resulting comb provides phase control of optical frequency markers across intervals of many hundreds of terahertz. Scientists can thus measure atoms and molecules by combining high-sensitivity, precise frequency control, broad spectral coverage, and high resolution in a single experimental platform.

Recent applications of cavity-enhanced direct frequency comb spectroscopy include sensitive and multiplexed trace-molecule detection for various species, as well as precise quantum control of atomic transitions via coherent pulse accumulations. More advanced spectroscopic and quantum control capabilities are being created by developing frequency comb sources in the deep ultraviolet and mid-infrared spectral regions. These distant spectral regions can in fact be coherently connected, thus in principle allowing the simultaneous study and control of vibrational and electronic molecular dynamics. The use of multiple frequency combs in pump-probe-type experiments has enabled increased resolution in both the temporal and spectral domain, and has for example yielded femtosecond time resolution of finely resolved optical properties in solids.

### *Real-time Chemical Kinetics*

A key recent success of frequency comb spectroscopy is its application to precise determination of real-time kinetics of important chemical reactions. The study of chemical reactions requires a comprehensive characterization of the dynamics of reactants, intermediates, and products. Because of their short-lived nature, reaction intermediates present the highest challenges. A new experimental capability has emerged and was recently applied to an important chemical reaction, OH+CO, under ambient conditions. This reaction has served as a benchmark system for kinetics and dynamics studies of complex-forming bimolecular reactions for the past four decades because of its importance in atmospheric and combustion chemistry (see Figure 5.7). With multiple elementary chemical reactions that produce two

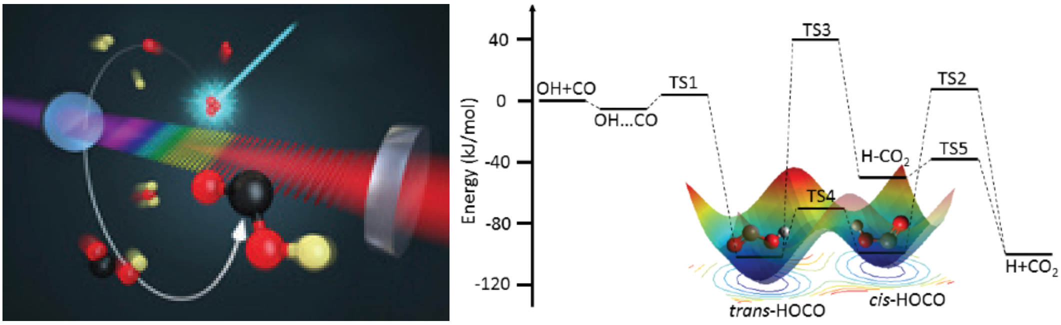

**FIGURE 5.7** An infrared frequency comb watches a reaction in real time. Bottom: Potential energy surface of the deuterated OH+CO reaction, showing the elusive reaction transients. Trans-DOCO and Cis-DOCO intermediates produced in the ambient reaction are observed simultaneously. SOURCE: The Ye Group and Steve Burrows, JILA.

transient intermediates (trans-HOCO and cis-HOCO) and products ($H+CO_2$) on a multidimensional potential energy surface, this reaction has been challenging to understand. Mid-infrared frequency comb spectroscopy allowed the first direct observation of trans-DOCO and cis-DOCO intermediates from OD+CO at thermal reaction conditions. (OD is a deuterated version of OH.) Together with measurements of $D+CO_2$ products, the experiment has allowed the full determination of rate coefficients for isomerization and branching ratios for all channels of this important multistep reaction.

### *Studying the Complex Structure of Large Molecules*

In Chapter 3, the exciting prospect of studying non-equilibrium dynamics of strongly interacting quantum systems is highlighted. Large and complex molecules present such an opportunity where a frequency-domain approach can reveal the complex structure that connects directly to the dynamics governing intramolecular energy flow between different degrees of freedom. This provides another important application opportunity for comb spectroscopy. Spectroscopic identification of larger room temperature molecules is nearly impossible because of spectral congestion. Cooling molecules to low temperatures drastically simplifies molecular spectra by enhancing the population of lower ro-vibrational states. The use of comb spectroscopy then opens the exploration of the complex energy-level structure of polyatomic molecules by providing a simultaneous map of the many relevant infrared transitions. In the case of $C_{60}$, the first quantum-state resolved spectroscopy was demonstrated in 2019. The observed transitions between individual ro-vibrational states reveal fundamental details of the quantum mechanical structure of $C_{60}$, including its remarkable icosahedral symmetry and nuclear-spin statistics. The possibilities for understanding and controlling complex quantum systems have thus been greatly advanced.

### Studying Dynamics Through Collision Physics

Many of the challenges involved in advancing our understanding of collisional phenomena boil down to the theoretical treatment of correlations, which arise in a variety of different contexts. In quantum chemistry, "correlations" are sometimes narrowly defined as electron-electron correlations that go beyond a Hartree-Fock independent electron model. But in fact, correlations are broader than this, as electron motion is correlated with nuclear motion in processes such as dissociative attachment or Penning ionization. At the experimental level, probing correlations is challenging because this normally requires multiparticle detection in coincidence, which leads to low count rates. Increasingly complex reactive processes can now be studied experimentally, through the enhancements over the years of technologies such as COLTRIMS and the so-called reaction microscope.

### Penning Ionization

A prominent example of a fundamental study involving correlation between electronic and nuclear motions in a small molecule, at the interface between chemical physics and AMO physics, is the challenging process of Penning ionization. This is a complex dynamical process in which an excited atom collides with a neutral atom or molecule, and leads to ejection of an electron, producing a positively charged atomic or molecular ion. Penning ionization has been observed and studied theoretically for decades, but until recently, with comparatively limited experimental evidence for the quantum mechanical nature of this process. In a remarkable experimental advance, it has now become possible to study this process in a low-temperature collision, below 1 degree Kelvin for excited helium atoms colliding with molecular hydrogen. In this regime, quantum mechanical resonances have been observed for the first time for such a complicated rearrangement collision.

### Reactive Processes Involving Physics: Topological Physics

Examples of excellent progress in the past decade include far better understanding of reactive processes that involve topological physics, which include physics related to conical intersections. In ultracold AMO physics context, as in condensed-matter physics, the word "topological" is often used to refer to many-particle phases of matter, but even systems with a few electrons and atoms involved exhibit topological features in their quantum mechanical behavior, especially in the context of reactive collisions. For instance, Jahn-Teller and Renner-Teller systems in molecular physics inherently involve correlated electron and nuclear degrees of freedom, and in some cases, Rydberg state interactions as well. Now calculations of the dissociative attachment process, such as electrons colliding with an ammonia molecule ($NH_3$) to produce an atomic hydrogen negative ion ($H^-$), can be carried

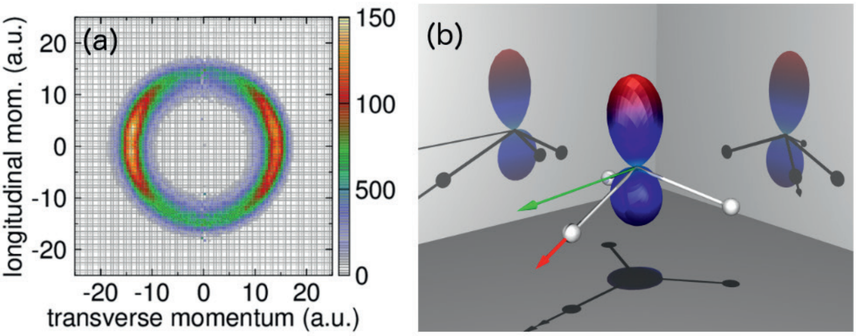

**FIGURE 5.8** $H^-$ production from $NH_3$. (a) Measured momentum distribution at 5.5 eV electron energy. (b) Calculated attachment probability as a function of incident electron direction in the molecular frame plotted as a surface, with rods showing NH bonds, and red and green arrows showing relevant recoil axes, discussed in the reference. SOURCE: Reprinted figure with permission from T.N. Rescigno, C.S. Trevisan, A.E. Orel, D.S. Slaughter, H. Adaniya, A. Belkacem, M. Weyland, A. Dorn, and C.W. McCurdy, Dynamics of dissociative electron attachment to ammonia, *Physical Review A* 93:052704, 2017, https://doi.org/10.1103/PhysRevA.93.052704; copyright 2017 by the American Physical Society.

out and tested in great detail by comparison with experiment. This exemplifies many advances of both theory and experiment to be able to measure specialized properties such as the angle of escape of the $H^-$ ion by using COLTRIMS and related techniques (see Figure 5.8). (See also the Chapter 3 section on Topological Matter with Cold Atoms for the role of topology in ultracold science contexts.)

### Broad Impact of Collision Dynamics Studies

While collision physics has tremendous intellectual challenges remaining—for example, to achieve a deeper understanding of reactions involving polyatomic molecules—there are additional strong practical motivations for advancing theory and experiment in this arena. The following examples showcase some of those subjects in need of better understanding of collision physics, especially reaction rates in a variety of environments:

- Impact on astrophysics: Extensive experimental and theoretical headway has emerged from studies of electron collisions with a variety of hydrogen-rich molecules that are very important in astrophysical environments—molecular ions like $HeH^+$, $H_2^+$, $H_3^+$, $CH_3^+$, $NH_4^+$, to name just a few. There is now an opportunity to build on this progress by tackling systems that would have been unimaginably complicated to consider treating theoretically, just one or two decades ago.

  One impressive development in experimental studies of low-energy small-molecule reactive collisions involving molecular ions, electrons, and neutral atoms or molecules has been the emergence of cryogenic storage rings (CSRs). The poster child for this technology is the CSR that recently became operational in Heidelberg, which is capable of cooling molecular target ions down to around 10 degrees above absolute zero, and is thus able for the first time to accurately mimic conditions in many astrophysical environments such as interstellar clouds.

Likewise, ion-atom collisions leading to charge-exchange processes emitting X rays that are detected by space-based telescopes can yield information on both the projectile and the target. Highly energetic events such as in the solar wind or supernova explosions lead to highly charged ions propagating through space. When these ions encounter neutral atoms, they can readily capture one or more electrons from the atom. The preferential route is via velocity matching, and so the electrons are likely to be captured to an excited state, which then decays by X-ray emission. The observation of the resulting X rays tells us their source ion and also the target atom. Accordingly, X-ray space-based telescopes are observing the emission of such charge-exchange processes and yielding information on the ingredients of their origin. The charge-exchange process is rather challenging to calculate due to its two-center (ion and atom) nature. A quantitative description of charge-exchange processes is possible for relatively simple ions and atoms, but can also be exceeding complicated.

- Plasma *modeling* of fusion plasmas such as those in the International Thermonuclear Experimental Reactor (ITER): The goal of the large-scale ITER project is to create abundant energy via nuclear fusion with the fuel being derived from seawater. While the building stage is now in full swing, there are still many uncertainties in energy balances inside the fusion plasma. As diverters will be made from tungsten, such impurities in the plasma will lead to radiative losses. There will also be other partially ionized impurities in the plasma that will also lead to radiative losses. Quantum collision theory is necessary to make accurate estimates of all of the radiative losses and free electron production due to ionizing collisions.
- Ion scattering on soft tissue to determine the stopping power of ions in the body for the purpose of ion therapy treatment of cancer: In the past decade or so, a new cancer treatment modality has been developed known as hadron therapy. The idea is an extension of proton therapy, namely to bombard tumors with even heavier projectiles such as carbon ions, and utilize the Bragg peak to destroy the tumor without affecting the healthy cells surrounding it. Many children have had their brain cancers completely cured with hadron therapy without the typical severe side-effects associated with conventional X-ray radiation therapy. The key aspect is to accurately calculate the stopping power of heavy ions in soft tissue, with liquid water

being a reasonable starting point. As the therapy is extremely expensive, the goal is to broaden its applicability to organs that may be moving due to the breathing of the patient during the therapy application. The determination of accurate stopping powers for ions is vital to ensure that the Bragg peak occurs at the tumor, and so away from healthy tissue.

- Positronium scattering on antiprotons to form antihydrogen: Further experimental progress toward understanding antimatter and questions about possible CPT violation, as is addressed in Chapter 6, requires greater numbers of antihydrogen atoms to be created. One technique for antihydrogen creation is guided by calculations of positronium (Ps) interactions with antiprotons. It has been shown that a rapid increase in antihydrogen production can be obtained via laser-excitation of Ps to utilize excited states, but the scaling is not as simple as classically expected. Generally, quantum collision theory will continue to provide guidance on the various mechanisms for producing antihydrogen.

### The Future of Frequency Domain Studies of Dynamics and Correlations

Many challenges remain in the field of collision physics, to treat more complex open-shell atoms, ions, and molecules and their reactivity, with or without external fields present. These are challenging problems that require a community of theoretical and experimental experts and capabilities. These involve quantal, semiclassical, or in some cases classical treatments of atomic or molecular energy levels or potential-energy surfaces, and of collisional dynamics such as electron-atom or electron-molecule scattering, ion-atom collisions, and atomic or molecular photoionization. It is imperative that the AMO community continue to invest in these capabilities, which impact so many other different fields in addition to having fundamental interest and importance in their own right.

Also in the frequency domain, with the revolutionary impact on precision metrology and ultrafast science brought by the recent development of optical frequency combs in the visible and mid-infrared spectral regions, we can naturally expect to extend this coherent spectral coverage to the extreme ultraviolet (XUV) ends of the spectrum. Ultrashort, ultraintense laser pulses at a high repetition rate can be frequency converted from visible to the VUV and XUV regions through high harmonic generation inside a femtosecond enhancement cavity. When the optical coherence from pulse to pulse is maintained, a frequency comb in the XUV spectral region can be generated, providing exceptional phase coherence for high-resolution spectroscopy, precision measurement, and quantum control. This is one of the best examples highlighting the advantage of joint control in both the time and frequency domains for optical fields.

## NOVEL PHYSICS WITH EXTREME LIGHT

As described in Chapter 2, the past decade has seen the appearance of a number of extreme light sources. XFEL facilities around the world have welcomed their first user experiments, including in the United States, Europe, and Asia. And Petawatt laser facilities continue to expand the limits for the highest intensity possible, with the European ELI project expected to reach intensities of $10^{23}$ W/cm$^2$ in the near future. This chapter ends with a brief discussion of the exciting physics that can be done using such light sources, spanning dynamics in AMO and beyond.

### Extreme Physics with XFEL Laser Light

XFEL sources provide coherent laser pulses of X-ray light with record-setting intensities and pulse durations. A number of XFEL experiments in this first decade have been performed on AMO systems, addressing fundamental questions and characterizing the capabilities of the light source. The sections above have described the capabilities enabled by the short duration of these pulses for dynamical studies. Other types of studies are enabled by the extreme intensity of these light sources.

One example of such studies is extreme ionization. The number of X-ray photons in a ~100 fs pulse from the Linac Coherent Light Source (LCLS) is so large compared to previous third-generation light sources that it is possible to strip the majority of electrons from small atomic or molecular systems. Early LCLS experiments on such extreme ionization of rare gas atoms (leading to $Ne^{10+}$, $Ar^{12+}$, $Xe^{36+}$) demonstrated that sequential, multi-step single-photon absorption by far dominates over direct multiphoton processes, even at the high intensities. In addition, the stripping away of electrons radically differed from intense optical pulses. In the latter case, valence electrons are removed sequentially, while intense X rays strip electrons from the inside out. In fact, the X-ray ionization is so rapid that it competes on the natural Auger time scale. More recently, researchers have shown that extreme ionization of small molecules is different from that of isolated atoms, and it can lead to the formation of a so-called molecular black hole (see Figure 5.9). This is because in a molecule, a charge imbalance created by X-ray ionization on one end of the molecule can be mitigated by electrons donated from the other end of the molecule. This charge transfer process is fast enough that it takes place even during the ultrashort (~100 fs) LCLS pulse, and means that more electrons can be removed from the molecule than from the group of individual atoms constituting the molecule. The interpretations of these experiments have been aided by large-scale calculations developed to describe the extremely fast ionization and rearrangement dynamics taking place during the X-ray pulse. These calculations combine quantum chemistry calculations of electronic structure with the coupled solutions of millions of equations describing the coupling between electronic states via transitions and decay.

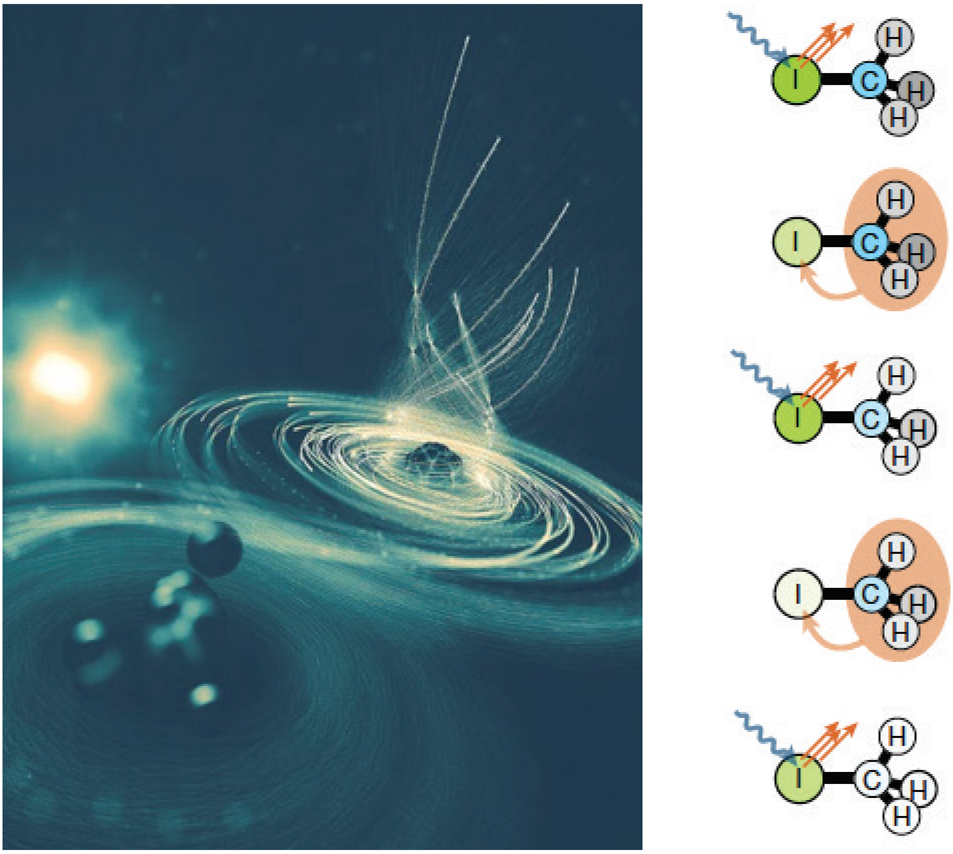

**FIGURE 5.9** The left picture illustrates how the extremely intense X-ray laser light removes so many electrons from the iodine (upper-right) end of a molecule that electrons get pulled in from the other (lower-left) end of the molecule, acting like an electromagnetic equivalent of a black hole. The process is illustrated schematically on the right: The X-ray photons (blue) can knock out multiple electrons from the iodine atom. Electrons from the methyl ($CH_3$) group will then be attracted to the positively charged iodine end of the molecule (orange arrow), somewhat replenishing the missing electrons from the iodine end. The X-ray pulse is so short that the molecule does not have time to dissociate, and so intense that the ionization from and replenishing of the iodine atom can happen multiple times before the pulse ends, leading to a highly charged molecular ion with electrons missing from both the iodine and the methyl end of the molecule. SOURCE: *Left:* See DESY, “X-ray Pulses Create ‘Molecular Black Hole,’” News, June 1, 2017, http://www.desy.de/news/news_search/index_eng.html, courtesy of DESY/Science Communication Lab. *Right:* Adapted from A. Rudenko, L. Inhester, K. Hanasaki, X. Li, S.J. Robatjazi, B. Erk, R. Boll, et al., Femtosecond response of polyatomic molecules to ultra-intense hard X-rays, *Nature* 546:129, 2017.

The extreme intensity of these novel sources also enables nonlinear optics in the X-ray regime. It is notoriously difficult to induce nonlinear optical processes in the X-ray spectral region, and only recently have low-order nonlinear optical processes such as second harmonic generation been observed experimentally. This is because nonlinear optical processes rely on a nonlinear response in some material, which is much weaker in the X-ray region than in the visible region. This means that the high X-ray intensities provided by XFELs provide an opportunity for studying X-ray nonlinear optics. Recent experiments have demonstrated two-photon atomic ionization of core electrons and nonlinear Compton scattering of X-ray photons in a solid target. Surprisingly, in the latter case, the researchers found that they could not explain the final photon energy of the scattered photon with the standard, semi-classical descriptions of Compton scattering. This finding illustrates how little is known about how matter interacts with intense X-ray fields in particular, and with extreme light fields more generally, and points toward the need for future studies.

### Reaching Beyond AMO Science Using Petawatt Laser Sources

The recent report on opportunities in intense ultrafast laser science[1] details the current and future scientific opportunities in this field, so here the committee gives only a brief overview. The applications of super-intense laser light have a broad reach with the potential to impact astrophysics, nuclear physics, materials science, and medical applications among others. For example, intense-field generated high-density plasmas containing relativistic particles, and their interaction with the electromagnetic field, are of interest in astrophysics for laboratory-scale investigations of the physics of exotic objects such as gamma-ray bursts, giant planets, and pulsar winds. Likewise, secondary sources of high-energy photons, protons, electrons, or neutrons that can be generated at very high laser intensity can be of interest to both nuclear physics and provide table-top rather than accelerator-size environments for experiments. These secondary sources have also shown a lot of promise for medical applications in both imaging and radiotherapy treatment, and for national security.

### Future of Applications of Extreme Light Sources

The field of short-wavelength nonlinear optics is only just opening up. With next-generation HHG sources of intense XUV light, and current-and-next generation XFEL sources of intense soft and hard X-ray light, we will be learning much more about the nonlinear response of atoms, molecules, and solids to intense short-wavelength radiation. The semiclassical model for the interaction of matter

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[1] National Academies of Sciences, Engineering, and Medicine, 2018, *Opportunities in Intense Ultrafast Lasers: Reaching for the Brightest Light*, The National Academies Press, Washington, DC.

with intense infrared laser light has been hugely influential in guiding experimental and conceptual progress in ultrafast and strong-field AMO science. It is an open question as to where the strong-field limit lies in the X-ray regime and in what way it will shape the development of new experiments and concepts. While it is unlikely that one-electron tunnel ionization would ever be dominant, a strong-field response in the X-ray regime could for instance involve a collective, many-electron response that would necessitate thinking beyond single-active-electron physics.

Another extreme-light setting for a "semiclassical" or recollision model is that of ultrarelativistic electrons—for example, created by ultra-intense, next-generation PW lasers—and their parent ions. The so-called Schwinger limit (above $10^{29}$ W/cm$^2$) is when the vacuum becomes unstable to electron-positron pair production, and the "classical" trajectories of charged particles will be completely disrupted even by single-photon emission. In analogy with strong-field atomic physics, coherent recollisions will become important as the electron kinetic energy greatly exceeds its rest mass. As discussed in Chapter 2, the Schwinger limit is not reachable with present-day lasers, but may be within reach in the next decade, potentially via collision of focused petawatt laser beams with ultrarelativistic electrons.

## FINDINGS AND RECOMMENDATIONS

In this chapter, the committee discussed the study of dynamics spanning the attosecond to the microsecond time scale, and how to access it in both the time domain and the frequency domain. The committee has discussed current and future progress in the making of time-domain molecular movies, spanning attosecond, coherent electron dynamics, through femtosecond molecular dynamics and beyond. It has been shown how improved resolution in the time domain, provided by modern ultrafast light and electron sources, has enabled fundamental investigations of time delays in photoionization, charge migration in molecules, and dynamics near conical intersections that are foundational not just to AMO physics, but also to materials science, chemistry, and photobiology. The unprecedented intensity available from XFELs has finally put time-resolved imaging of individual molecules within reach and has opened new fields of multiphoton and nonlinear X-ray physics, where the behavior of matter under extreme conditions can be explored. The committee also discussed how improved sensitivity in the frequency domain, both that provided by modern frequency-comb light sources, amurind by advances in collision physics, allows complementary studies of dynamical processes.

> **Finding:** This is a unique time in ultrafast science due to the ubiquity and controllability of ultrafast light sources spanning the terahertz through the hard X-ray regime. The development and application of these sources have driven much of the progress described in this chapter.

**Finding:** Control of ultrafast electron dynamics in molecular and condensed-phase systems has significant potential for impact well beyond AMO science, including at the technological and industrial levels. Likewise, continued development of molecular movies will drive advances at the fundamental level, and promises societal benefits through improved understanding of photo-driven biological processes.

**Finding:** Continued progress on these challenges will require the combined expertise of multiple principal investigators (PIs) and mid-scale infrastructure, either because they involve advanced facilities with many different elements, or because they are inherently multidisciplinary in nature, covering AMO, condensed-matter physics, chemistry, laser technology, and large-scale computation. Funding mechanisms similar to the Physics Frontiers Centers or Multidisciplinary University Research Initiatives, in which multiple PIs from experiment and theory work toward a common goal, are crucial.

**Key Recommendation: U.S. federal agencies should invest in a broad range of science that takes advantage of ultrafast X-ray light source facilities, while maintaining a strong single principal investigator funding model. This includes the establishment of open user facilities in mid-scale university-hosted settings.**

**Finding:** There has been widespread use of data typically gathered in collision physics, which are needed for applications and analysis in astrophysics, plasma physics, and nuclear medicine among others, as well as a decline in university-supported collision physics groups.

**Recommendation: National laboratories and NASA should secure the continuation of collision physics and spectroscopy expertise in their research portfolios.**

# 6

# Precision Frontier and Fundamental Nature of the Universe

## INTRODUCTION

One hundred years ago scientists believed they understood the fundamental principles of nature: most scientific problems seemed to have been solved. Newtonian mechanics, electromagnetism, and thermodynamics served the needs of world technology, and the progress in comparison with the previous century seemed staggering. Yet there were hints of new physics—atomic spectra, the photoelectric effect, and mysterious X rays; and a few now-famous names already had said the word "quantum." No one in 1919, or even 1959, could have imagined what quantum mechanics would bring to the world, and how much of our technology would depend on understanding the nature of atoms, light, and their interaction. In the tremendous success of quantum mechanics, general relativity, and the Standard Model (SM) of particle physics lies the danger—to think again that we understand the fundamental principles of nature. The glaring signs of new physics are here again, just as they were in 1919: the universe of the SM should have too much antimatter for us to ever come into existence and the SM particles only account for less than 5 percent of it. It is our great hope that we are standing again on the brink of the new era just before the new discoveries stemming from finding solutions to these problems. As it was with quantum mechanics, one cannot even begin to imagine what new technologies these new discoveries will bring.

We now live fully in the world of the quantum. The extraordinary advances in control of quantum matter and light discussed in previous chapters have generated transformative tools for precision measurement. It is remarkable that once again it is the study of atoms and light, just as it was a 100 years ago, that enables experiments that can probe the most basic laws of nature, and that allow us to gain a fundamental understanding of the physical universe. What atomic, molecular, and optical (AMO) science brings to the table is the availability of precisely controlled ultracold atoms, vast improvements in precision time and frequency metrology, and measurement techniques such as atomic magnetometry and interferometry. These experimental frontiers are coupled with recent advances in first-principles atomic and molecular theory. Together, these tools now allow novel AMO-based tests of the fundamental laws of physics with unprecedented sensitivity. The advances in precision have been so striking in the past decade that the question naturally arises: Do the fundamental laws of physics as we know them hold at the level of experimental precision now available? The potential for paradigm-shifting discoveries is fueled by exceptional versatility, inventiveness, and rapid development of AMO experiments, supported by continuous technological advances described in other chapters.

Thus, on the one hand AMO research, with its capability for precision measurement, is likely to transform our view of the universe—competing and in some areas overmatching what can be achieved with accelerators. For example, AMO-based searches for the electron electric dipole moment (eEDM) have already constrained new particles beyond the energy scale reachable by present colliders. The fantastic achievement of detecting gravitational waves was also enabled by quantum technologies. Moreover, the first prototype of a new type of gravitational wave detector based on matter waves has just been approved for construction. New searches for dark matter (DM) are ongoing using all the AMO precision tools discussed in this chapter—including atomic clocks, interferometers, and magnetometers—exploring DM candidates that cannot be discovered with other technologies. Atom interferometry has provided the best limit on some possible dark energy scenarios.

On the other hand, many of the same tools being used to probe fundamental physics are also extremely useful as real-world sensors. The latter include the best clocks, magnetometers, gravitometers and gravity gradiometers, as well as inertial sensors. These are critical to industry, healthcare, and military applications, as well as to further explorations in basic and applied sciences. Such sensors are discussed in the sections below, together with their applications, both real-world and in fundamental physics. We emphasize that it is the inherently quantum nature of all the sensors described here that enables this level of precision. Most of these sensors rely on coherent superposition and exquisite control of the quantum states. Thus precision measurement, and its correlate of sensing, are in fact part of the quantum technological revolution.

This chapter begins with a consideration of unresolved fundamental problems about the nature of our universe that AMO enables one to address. Next are sections on precision measurement technologies and theory advances that are used to address these questions. This leads into sections describing specific experiments aimed at answering these questions. The chapter concludes with a discussion of future directions and opportunities. For more in-depth exploration of parts of this topic the committee refers the reader to an extensive review article, "Search for New Physics with Atoms and Molecules," containing approximately 1,100 citations to mostly recent work.

## CRISIS OF MODERN FUNDAMENTAL PHYSICS

We live in an exciting time for fundamental physics. All the particles predicted by the so-called Standard Model (see Figure 6.1), which describes the fundamental particles that make up matter and the fundamental force carriers, have been detected. The full description was experimentally completed with the discovery of the Higgs boson at the Large Hadron Collider (LHC) at CERN in 2012.

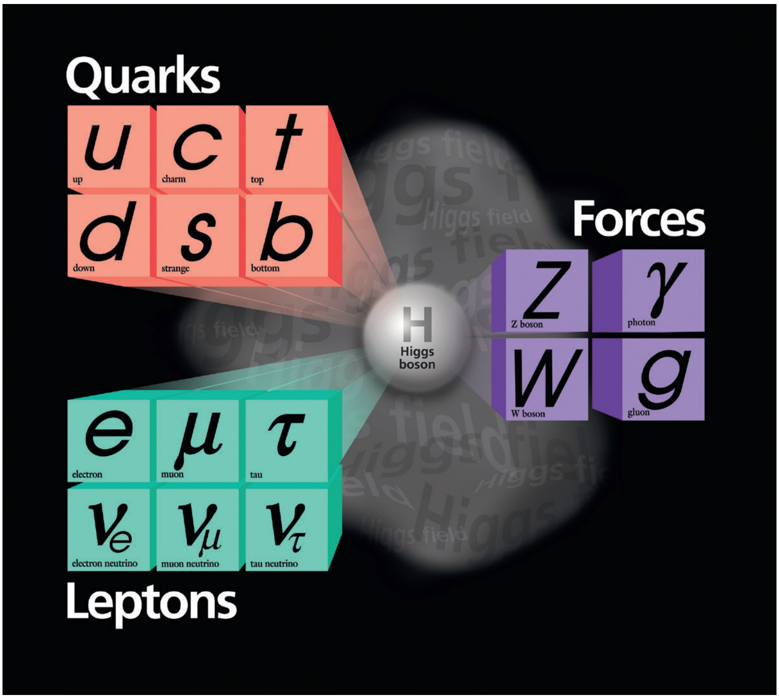

**FIGURE 6.1** The Standard Model (SM) of elementary particles includes quarks, leptons, force carriers of strong, weak, and electromagnetic interactions, and the Higgs boson. The SM has been very successful in describing, as well as predicting, virtually everything seen in nuclear and particle physics. Nevertheless, as a "complete" theory it has major issues—many key features of the universe remain unexplained. SOURCE: Fermi National Accelerator Laboratory; see https://commons.wikimedia.org/wiki/File:Standard_Model_From_Fermi_Lab.jpg.

Nevertheless, we now know that the SM describes only a very small fraction of the universe's composition: from the 2015 results of the Planck Mission to study the cosmic microwave background radiation, we know that our present universe is 69 percent dark energy, 26 percent DM, and only 5 percent ordinary (SM) matter. The DM is observed only via its gravitational interaction; its composition remains a mystery, although evidence for its existence dates back to the 1930s. Its apparent existence is confirmed by numerous studies of astronomical objects. But it does not fit within the SM. Decades of investigation have not identified the nature of DM, although many "candidates" are theoretically hypothesized. So far, we have learned only what most of it is not—namely, none of the particles of the SM. All of the AMO precision tools discussed in this chapter—atomic clocks, interferometers, and magnetometers—are now being used as DM detectors, and many DM candidates can be probed only with precision experiments.

The existence of "dark energy" is inferred from studies of Type I supernovae, demonstrating that the expansion of the universe is now accelerating, something possible only if our universe contains an unknown kind of energy that effectively acts as repulsive gravity. The existence of DM and dark energy provides a very strong motivation to search for new particles (or their associated fields) beyond those described in the SM. Atom interferometry provides the strongest limits on some dark energy candidates.

In a sense, the SM is inconsistent with the very existence of our universe: it cannot account for the observed imbalance of matter and antimatter, and therefore cannot explain how matter survived the annihilation with antimatter after the Big Bang. Searches for the electric dipole moments of atoms and molecules described in this chapter test theories aimed to explain this asymmetry.

Another major fundamental problem is the nature of gravity. As one can see from Figure 6.1, the SM does not include gravity. Despite many decades of effort, all attempts to unify gravity with the other fundamental interactions remains unsuccessful, and there is no understanding of why gravity is so weak in comparison with the other fundamental forces.

These shortcomings of the SM have long been known. However, the rapid improvement of the precision tools of AMO physics during the past decade place us at an extraordinary point in time for physics discovery. While one can search for new particles directly with large-scale collider experiments at the high-energy (TeV = $10^{12}$ eV) scale, such as those carried out at the LHC, new physics may very well be observed via low-energy precision measurements based on AMO science. In many theories that have been proposed to go beyond the Standard Model (BSM), Lorentz invariance, universality of free fall, local position invariance, constancy of fundamental constants, and the like, no longer need to hold. Thus the discovery of their violation with the kinds of techniques described in this chapter will be a first glimpse into the nature of BSM physics. In addition, AMO measurements test predictions of new physics theories—non-observation of electron EDM rules out or restricts classes of such theories, and other AMO experiments restrict possible DM candidates.

## PRECISION MEASUREMENT TECHNOLOGIES

### Atomic Clocks

Atomic clocks were briefly described in Chapter 2. Here, the committee focuses on new prospects in clock development, as these are particularly important for probing fundamental physics questions. Systematic uncertainties of $1 \times 10^{-18}$ have now been demonstrated with clocks based on both neutral atoms trapped in an optical lattice and on single trapped ions, as shown in Figure 6.2. Optical lattice clocks now demonstrate extraordinary statistical uncertainty of $5 \times 10^{-19}$ in 1 hour.

Atomic clocks are uniquely sensitive to a number of new physics signatures. For example, variation of the fine-structure constant will cause changes in optical clock transition frequencies, with the amount of change dependent on the clock transition. Microwave clocks (as well as some novel future clocks described below) are sensitive to the variation in other constants involving ratios of particle masses. Therefore, monitoring ratios of two (different) clock frequencies over time allows one to search for the variation of fundamental constants. Light DM can cause oscillatory or transient changes of the fundamental constants and, therefore, clock

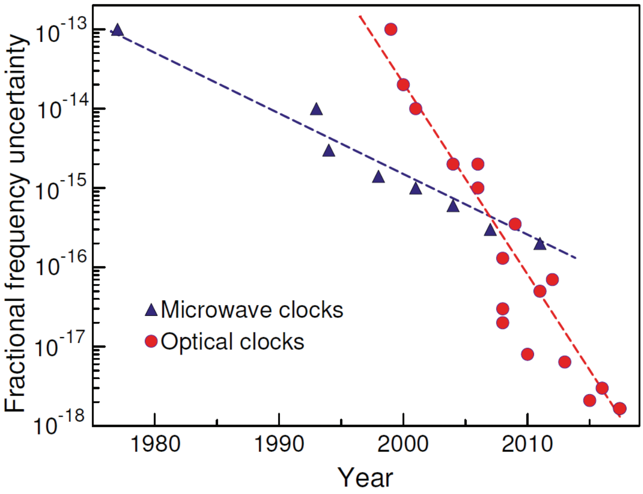

**FIGURE 6.2** The evolution of fractional frequency uncertainties of atomic frequency standards based on both microwave (Cs clocks) and optical transitions. SOURCE: From Rev. Mod. Phys. 90, 025008 (2018), with new (last) data point added.

frequencies. The presence of such signals can be extracted from clock-comparison experiments. The advances in atomic clocks over the past decade have already enabled improved tests of the constancy of the fine-structure constant and proton-to-electron-mass ratio, several orders of magnitude improved tests of Lorentz invariance, and new applications of clocks to DM detection as described in the section later in this chapter, "Searches for New Physics Beyond the Standard Model."

Considering that the gravitational redshift is $1 \times 10^{-19}$ for a 1 mm height change on Earth, it is tantalizing to think of the future scientific possibilities when we improve clock performance to, say, the $1 \times 10^{-21}$ precision level, when the gravitational redshift on clock atoms separated by a mere 10 μm can be detected. Such capabilities will be invaluable for relativistic geodesy and testing quantum mechanics in curved spacetime.

To reach this exciting new regime, advances in ultrastable lasers and precise control of quantum states of many atoms will be necessary. Furthermore, exciting new opportunities have emerged for the next generation of state-of-the-art precision quantum metrology, such as harnessing the interactions between atoms to create and manipulate interparticle correlations and entanglement for precision measurements of time, frequency, and space.

Such work has already started with the development of a three-dimensional (3D) optical lattice with Sr atoms forming a Mott insulator. This configuration suppresses effects of atomic contact interactions, and extends interrogation times to beyond 10 s. Even with atoms pinned in a 3D lattice, long-range dipolar interactions can degrade clock precision, and give rise to an important systematic effect. Understanding and controlling both the real and imaginary parts of dipolar interactions will be crucial for the next generation of clocks. New techniques, such as using an adjustable optical lattice, or an array of optical tweezers, to configure these many atoms in a spatially ordered and stationary regime, could extend the coherence time to the limit of the Sr excited state lifetime of more than 100 seconds.

In addition to further development of the current clocks, new clocks are being proposed and developed that are much more sensitive (by a factor of 100 to 10,000) to fundamental physics questions. As mentioned earlier, these promise to enable measurements such as variation of fundamental constants, as well as tests of local position invariance, and DM searches. These are described later in this chapter.

Highly charged ions (HCIs) offer extremely narrow optical transitions that are less sensitive to some of the external perturbations as compared to current atomic clocks. These should have a high sensitivity to the variation of the fine-structure constant due to relativistic enhancement. Development of high-precision atomic clocks requires cooling, trapping, and precision control of the various atomic species. Direct laser cooling, used for neutral atoms and singly charged ions, is impossible for HCIs, which lack the necessary fast-cycling optical transitions. In 2015, a breakthrough demonstration was reported of sympathetic cooling of $Ar^{13+}$ down to below 100 mK, by using a laser-cooled $Be^+$ Coulomb crystal in a cryogenic Paul trap. In 2018, quantum logic spectroscopy of $Ar^{13+}$—in which a $Be^+$ ion, trapped together with the spectroscopy ion, provides sympathetic cooling, control, and readout of the internal state of the spectroscopy ion—was demonstrated at PTB, Germany. This new development opens the pathway toward rapid development of HCI clocks.

In contrast to atomic transitions, nuclear transition frequencies are typically many orders of magnitude higher than those accessible by lasers, with the unique exception of a long-lived nuclear transition that occurs between an excited state (isomer) of the $^{229}$Th isotope and the corresponding nuclear ground state. Designing a clock based on this nuclear transition, with a wavelength of 150(3) nm, is particularly attractive due to the suppression of field-induced frequency shifts, since the nucleus interacts only via the relatively small nuclear moments and is highly isolated from the environment by the electron cloud. The existence of the isomer was definitively confirmed in 2016 by a European collaboration. Further laser spectroscopy investigation of the hyperfine structure of the isomer yielded the first nuclear properties. These recent experimental milestones have provided a solid base for progress toward the accurate measurement of a transition frequency, and realization of an actual nuclear clock. Two different types of nuclear clock designs have been proposed, one based on trapped ions and another on a solid-state system in which Th is implanted in crystals transparent to radiation in the vacuum-ultraviolet range. It has been suggested that such a nuclear clock would be enormously more sensitive (by five orders of magnitude) to the variation of the fine-structure constant and quark masses than all atomic clocks currently in operation.

Preparations are under way for the development of HCI clocks and nuclear clocks. Efforts in the United States to pursue these opportunities in novel clock development are also underway.

### Quantum Metrology Using Correlated States

The performance of many precision sensors is limited by fundamental noise properties dictated by quantum mechanics. For example, the frequency stability of atomic time standards is currently limited by so-called quantum projection noise, associated with detection of the number of atoms in a given clock output state. In this case, each atom behaves in a statistically independent way from all other atoms in the clock; in general, the sensor output is given by the statistics of an ensemble of independent, uncorrelated particles. However, it has been known for several decades that quantum mechanics in principle allows access to significantly improved performance if a suitably quantum correlated state is used for the sensor. In this case, particles no longer behave as statistically independent entities; rather, the quantum states of particles (e.g., the two atomic states comprising an atomic clock) become statistically correlated—entangled—across the entire ensemble. In the case of photons, quantum correlations lead to the squeezed states of light discussed in Chapter 2 and again later in this chapter. Amazingly, these correlations can be achieved in such a way that they may improve the noise performance of the sensor without fundamentally altering its function. The physically allowable improvements can be dramatic. For a sensor employing N particles prepared in an appropriately correlated state, the measurement precision can improve beyond the normal $N^{1/2}$ scaling. In principle, for an atomic clock with 1 million atoms, one may achieve a thousand-fold performance improvement beyond the standard quantum limit.

Broadly speaking, the performance of any precision sensor can in principle be improved with such methods. For example, an atom interferometer gyroscope that performs at a noise level suitable for aircraft navigation can, with such methods, achieve performance levels better than the very best strategic-grade gyroscopes used for submarine navigation. The detection noise performance—and thus the astrophysical reach—of a gravitational-wave detector can be likewise improved.

It is extremely challenging to produce the states that can yield the ultimate level of performance—the so-called Heisenberg limit. However, with recent advances in methods to control the quantum mechanical states of ensembles of particles, pioneering experiments in the past decade have already indicated the possible effectiveness of this approach. Since the methods needed to build the required correlated states for sensing are intimately connected with those exploited for quantum information processing, it is anticipated that substantial progress is likely in the coming decade. With sustained investment in basic and applied research in this area, it is likely that many classes of fundamental and applied sensors (e.g., magnetometers, clocks, accelerometers, gyroscopes, gravimeters, and gravitational-wave detectors) will see very significant performance improvement by adoption of these methods.

### Atom Interferometric Inertial Sensors

Atom interferometers exploit the quantum mechanical wave properties of matter to realize sensors and instruments analogous to optical interferometers. Progress in this field has been fueled by development of cold atomic sources, which offer precise control over the velocity, hence wavelength (via the de Broglie relation) of the interfering atomic particles. De Broglie wave interferometers for atoms were first realized in the early 1990s; the past decades have seen a significant growth in both the reach and capabilities of these instruments. For example, current atom interferometers realize atomic wave-packet separations of 0.5 m over temporal durations of 2 s by exploiting increasingly sophisticated atom/laser interactions to manipulate atomic center of mass wave-functions. These observations indicate the extraordinary level of control that can now be exerted on ensembles of atoms.

They provide stunning examples of the manifestation of quantum phenomena on macroscopic human scales. Such laboratory interferometers are now finding use in tests of gravitational physics, quantum mechanics, and in searches for physics beyond the Standard Model, as the science reach of tests like these is intimately linked with these aspects of our fundamental understanding. On the other hand, as supporting photonics technologies have matured, early laboratory-scale proof-of-concept demonstrations of inertial force sensing capabilities have matured into a class of field-deployed sensors for gravitational fields, gravity gradients, and rotations. The performance of these sensors is now beginning to compete favorably with existing state-of-the-art sensors. Related instruments have been recently used to make new measurements of the fine-structure constant through indirect observation of the momentum recoil of atomic wave-packets induced by photon scattering.

Atom interferometric inertial sensors derive a performance advantage compared to existing state-of-the-art sensors from the fact that atoms are superbly isolated from spurious non-inertial forces, and from the fact that precision laser sources are used to manipulate and control atomic wave-functions. These attributes enable new classes of high-accuracy sensors. For example, commercial atom interferometric gravimeters achieve $10^{-9}$ g accuracies, and atom interferometric gyroscopes have exceptional bias and scale factor stability. The noise performance of these sensors continues to improve as well-engineered high-flux atomic sources mature, as sensor noise performance is limited by the shot noise associated with the number of atoms detected in a given observation time. In practice, noise performance for well-engineered sensors meets and can exceed the performance of sensors based on other technologies. The combined noise and accuracy attributes of atom interferometric sensors makes them uniquely suited for applications such as, for example, precision inertial navigation.

In the coming decade, further advances are foreseen in the performance, integration, and size of fieldable sensors. For example, deployed gravity gradiometers with 0.01 $\mathrm{E/Hz}^{1/2}$ noise performance appear feasible. ($1\ \mathrm{E} = 10^{-9}\ \mathrm{s}^{-2}$; for reference, the gravity gradient due to the Earth's gravitational field, as measured on the Earth's surface is ~ 3,000 E.) Such sensors have national security applications in underground structure detection; and commercial application in oil and mineral exploration, in which structures and deposits are identified through their gravitational signatures. On the other hand, the performance of laboratory-based (versus fieldable) sensors is expected to continue to advance with improved atom optics and implementation of quantum metrology detection protocols. Lastly, space-based platforms are well suited to atom interferometric sensors, as these sensors benefit from the long free-fall times available in this environment. Recent development of space-based cold atom platforms (NASA Cold Atom Lab) suggests the possibility of future space missions. Applications of space-based inertial sensors include gravitational geodesy and gravitational wave detection, as well as fundamental gravitational physics experiments such as tests of the equivalence principle.

### Gravitational Wave Detection

Gravitational waves (GWs) were predicted by Einstein in 1916, as part of his General Theory of Relativity (GR). GR presented a completely new way of understanding gravity, not as a force between massive objects, but as the geometry of spacetime. In GR, massive objects cause the space around them to curve, and clocks near them to tick more slowly. When massive objects accelerate, spacetime ripples, and GWs are generated that can travel across the universe carrying information about their sources.

GWs are very weak; only compact masses moving at relativistic speeds radiate GWs with appreciable strength. Even some of the most violent collisions in the universe—mergers of neutron stars and black holes in the nearby universe—cause only the slightest ripples of spacetime here on Earth. As these ripples pass through a region of spacetime, they change spacetime distances L by an amount $\Delta L = h L$, where h is the amplitude of the GW. The GWs from a pair of neutron stars, comprising the densest matter known, merging with each other in a nearby galaxy would change kilometers-long distances between objects here on Earth by $\Delta L = 10^{-21} \times 1{,}000$ m $= 10^{-18}$ m, or 1/1,000th the size of a single proton. Consequently, for many decades after Einstein's prediction, the prospects for measuring GWs seemed grim—they were just too faint.

In the 1960s, with the invention of the laser and the discovery of neutron stars and black holes, the prospects for detecting these faint waves from real astrophysical sources began to seem within reach (see Box 6.1). A passing GW can be detected by measuring the spacetime distances between freely floating objects or "test masses." The test masses must be shielded from all external forces well enough that their motion is due to the GW. If laser light, with its exquisite precision, is to be used as the meter stick for measuring the spacing between the test mass, then the test masses must also double as mirrors.

### Quantum Engineering for Gravitational Wave Detectors

In Chapter 2, the committee introduced squeezed states of light—specially engineered quantum states where the noise is redistributed between the amplitude and phase properties of the light. Improving the sensitivity of laser interferometer GW detectors is an immediate and tangible application of squeezed states. Figure 6.3 shows the improvement to the noise performance of the Laser Interferometer Gravitational-Wave Observatory (LIGO) Livingston detector when squeezed states are injected. The approximately 30 percent improvement in strain

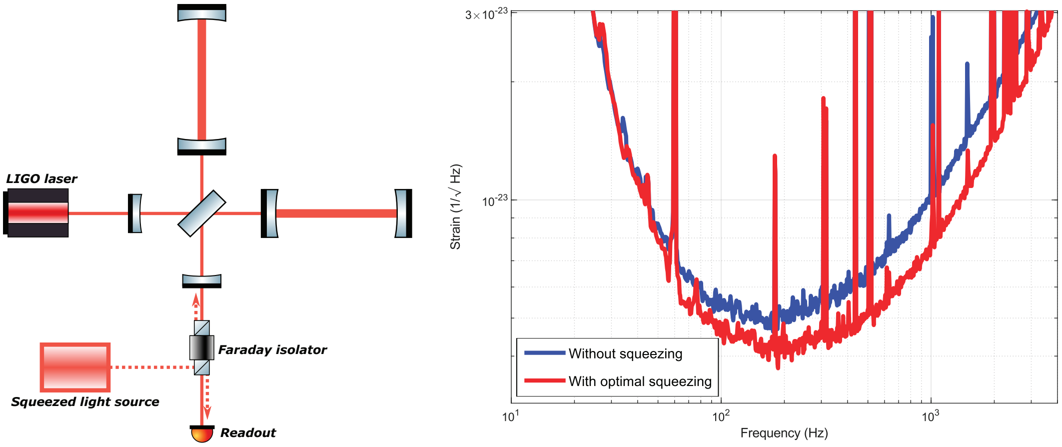

**FIGURE 6.3** Injection of squeezed states into the Laser Interferometer Gravitational-Wave Observatory (LIGO) detectors leads to improved sensitivity. Left panel: Squeezed states are generated with a sub-threshold optical parametric oscillator, where optical nonlinearity creates correlations between photons. The squeezed states are injected into the output (anti-symmetric) port of a LIGO interferometer; they propagate through the interferometer and exit the antisymmetric port along with the GW signal imprinted on the laser light that was incident through the symmetric port. The combined fields detected by the output photodetector can have noise lower than the shot noise limit without squeezing, as shown in the right panel. Right panel: Spectra of the noise limits of the Advanced LIGO detector at Livingston, Louisiana. The blue curve is the performance when no squeezed states are injected, and the red curve is with squeezing. Squeezing gives a roughly 30 percent improvement at frequencies with the most improvement, which should give more than a factor of 2 improvement in the rate of detections for Advanced LIGO. The line features are typically of power lines, calibration lines, and mechanical resonances. SOURCE: Maggie Tse/LIGO.

sensitivity should lead to a factor of 2 increase in the rate at which astrophysical sources may be detected.

## Gravitational Wave Observatories in Space

Just as the electromagnetic spectrum spans wavelengths from kilometers (radio waves) to picometers (gamma radiation), so also the GW spectrum spans 20 orders of magnitude in wavelength. Different sources radiate GWs at different wavelengths, depending on the physical processes underlying the radiation. Earth-based detectors like LIGO are sensitive to GWs of frequencies between 10 Hz and 10 kHz, typically radiated by compact objects that have a few times the mass of our Sun. Much heavier objects, such as supermassive black holes at the centers of galaxies, would radiate GWs at much lower frequencies, in the 10 to 100 mHz range. Terrestrial detectors are unable to observe GWs at these lower frequencies since vibrations on Earth are too large. Exploring the rich menagerie of GW sources at

### BOX 6.1
### Laser Interferometry for Gravitational-Wave Detection

The combination of mirror test masses and ultrastable lasers led to the conception of a bold experiment called LIGO—the Laser Interferometer Gravitational-Wave Observatory—that sought to directly measure gravitational waves (GWs) using precision optical interferometry. LIGO was funded by the National Science Foundation (NSF) over four decades, an investment that in 2015 realized two laser interferometers that had the precision to measure changes in the distances between mirrors that were 4 km apart at the level of $10^{-18}$ m. To reach this precision, LIGO uses many techniques of precision measurement and quantum optics that were developed as part of the extensive, diverse, and growing AMO science toolkit.

The imperative to continue to explore the universe with GWs, searching for new unknown objects, and gaining a deeper understanding of what we already see, is driving exploration and design of a new generation of laser interferometric GW detectors that will be capable of mapping out all merging black hole binaries in the observable universe. The design of these so-called third-generation instruments is pushing the frontiers of precision measurement, from lasers and optical technologies, to vibration control, to engineering new optical materials, to subquantum sensing techniques. This continuing development of new capabilities in precision measurement is the direct result of the interplay between the fields of atomic, molecular, and optical (AMO) science and GW detection.

Since the first detection in 2015 (see Figure 6.1.1), LIGO and its European counterpart Virgo, have published confirmed detections of GWs from 10 binary black hole mergers and one neutron star merger, as of Summer 2019. Unlike black hole collisions, where little or no light is given off, GW emission from neutron star collisions are followed by a spectacular light show, as neutrons fuse to make heavier and heavier elements. GW measurements of the neutron star merger by LIGO and Virgo triggered a massive observational campaign by telescopes worldwide, and the emitted light was observed at many wavelengths, from radio to infrared to optical to X rays to gamma rays. One of the great attractions of observing the universe with GWs is that they are emitted by objects that may not give off light, and so are undetectable using traditional telescopes. Even when they do emit light, as in the neutron star merger case, GWs provide complementary information that provides a much fuller understanding. These first GW discoveries are already changing our understanding of some of the most violent events in our universe.

lower frequencies motivates GW detectors in space. The most advanced in design is the Laser Interferometer Space Antenna (LISA), a European space mission that the National Aeronautics and Space Administration (NASA) partners in.

LISA comprises three satellites that are about 1 million kilometers apart and fly in a triangular formation, shooting laser beams from one to the other. Precise on-board clocks measure the time of arrival of laser beams to infer the spacetime distances, which would be modulated by passing GWs. Like LIGO, LISA uses a vast array of AMO tools, from ultrastable lasers and atomic clocks to quantum-noise-limited optical measurement. LISA technologies have been developed for the past

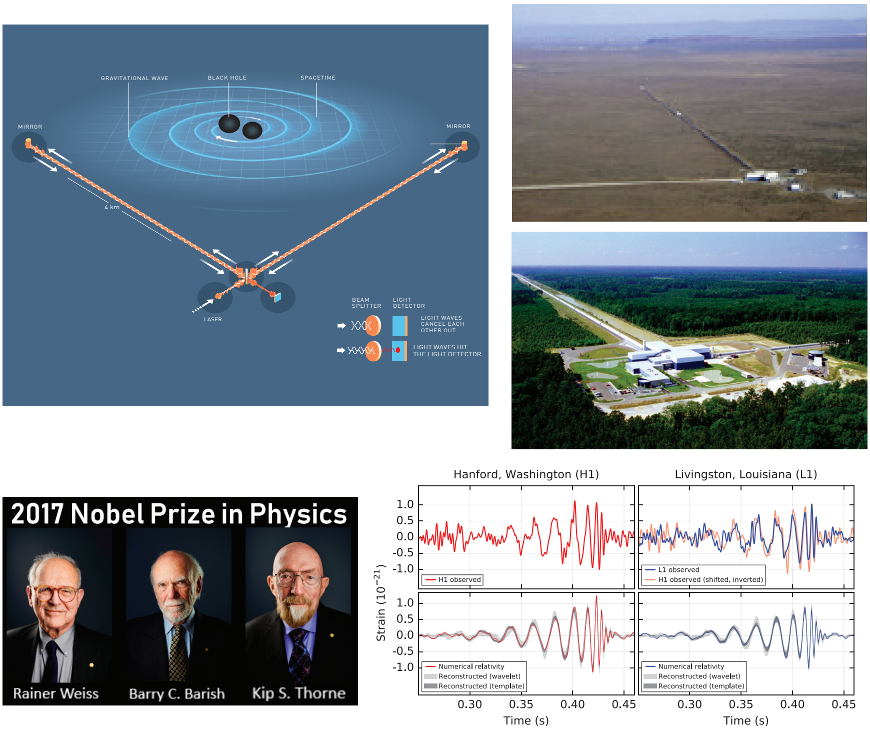

**FIGURE 6.1.1** Historic first detection of gravitational waves. *Clockwise from top left:* The precision optical measurement is made by detecting the interference between two light beams in the arms of a laser interferometer; aerial views of the LIGO observatories in Washington and Louisiana; the first gravitational wave signals from colliding black holes were observed by the detectors on September 14, 2015; the 2017 Nobel Prize in Physics was awarded to Rainer Weiss, Kip Thorne, and Barry Barish for "decisive contributions to the LIGO detector and the observation of gravitational waves." The success of LIGO can be directly attributed to long-term sustained funding by NSF over decades. SOURCE: *Clockwise from top left:* ©Johan Jarnestad/The Royal Swedish Academy of Sciences; Caltech/MIT/LIGO Lab; Nobel Media; Nergis Mavalvala/LIGO.

three decades, culminating in an important space test called the LISA Pathfinder mission. Following the spectacular success of the Pathfinder mission, which demonstrated that the spacecraft can be controlled to meet the stringent requirements on acceleration, LISA is now slated for launch in 2034.

### Matter Wave Interferometry for Future Gravitational Wave Detection

Laser interferometry is the most mature technology for GW detection, owing in no small part to decades of intellectual and financial investments. But it is not the only technology that can be used for GW detection. Advances in atomic physics and optical physics have provided tools that enable new classes of precision measurements, including GW detection. These tools include atom interferometry, as discussed in the previous section in the context of inertial sensing, where quantum mechanical interference of atomic de Broglie waves enables precise force measurements. The combination of atom interferometry and ultrastable lasers, which have led to a generational advance in the performance of atom-based sensors, has the potential to provide a novel method for GW detection in future decades.

In the atom interferometric approach, gravitational radiation is sensed through the gravitational wave-induced phase shifts on the propagation of laser beams between two spatially separated, inertially isolated, laser-cooled atomic ensembles. Momentum recoil associated with the interactions between the laser and atomic ensembles results in the concomitant interference of atomic wave packets. Functionally, the atomic ensembles serve as precision clocks that measure the flight time of light between the atom ensembles. In the case of space-based atom interferometric GW detectors, optical lattice clocks paired with conventional drag-free vibration isolation (e.g., in LISA Pathfinder) can also realize scientifically interesting strain sensitivity levels.

For ground-based configurations (see Figure 6.4), the atomic interferometric approach provides immunity to local seismic noise, and thus may enable detection of gravitational waves in the 0.3 Hz to 10 Hz frequency band. A 100 m prototype detector (MAGIS) is currently being built to evaluate the efficacy of this approach. This instrument also provides new detection modalities for ultralight DM. Related instruments are under development in France (MIGA) and China (ZAIGA).

The GW spectrum between 0.03 Hz and 10 Hz appears to be scientifically rich. The lower end of this range would allow observation of white dwarf binary mergers, while the higher frequency region (~1 Hz) is potentially a valuable region for searching for cosmological sources. Moreover, black hole or neutron star binaries may be observed in different frequency bands during their in-spiral, merger, and ring-down phases. Observations by LISA at tens of mHz, and future mid-band detectors operating at higher frequencies, could give predictions of the time and location of a merger event at tens of hertz in LIGO, which in turn would allow narrow-field high-sensitivity optical, X-ray, gamma ray, and other telescopes to point to observe the prompt emission during the actual merger. Since the sources generally emit for a long time in this mid-frequency band, they can be localized on the sky even by a single-baseline detector, since the detector will change orientation and position significantly during the time spent observing a single source. This can potentially lead to new, powerful cosmological probes.

Altogether, LIGO/Virgo and their descendent experiments, such as LISA, and future atom interferometry-based GW detectors, have the potential to cover a large part of the GW spectrum. As a result, we should be able to map out astrophysical

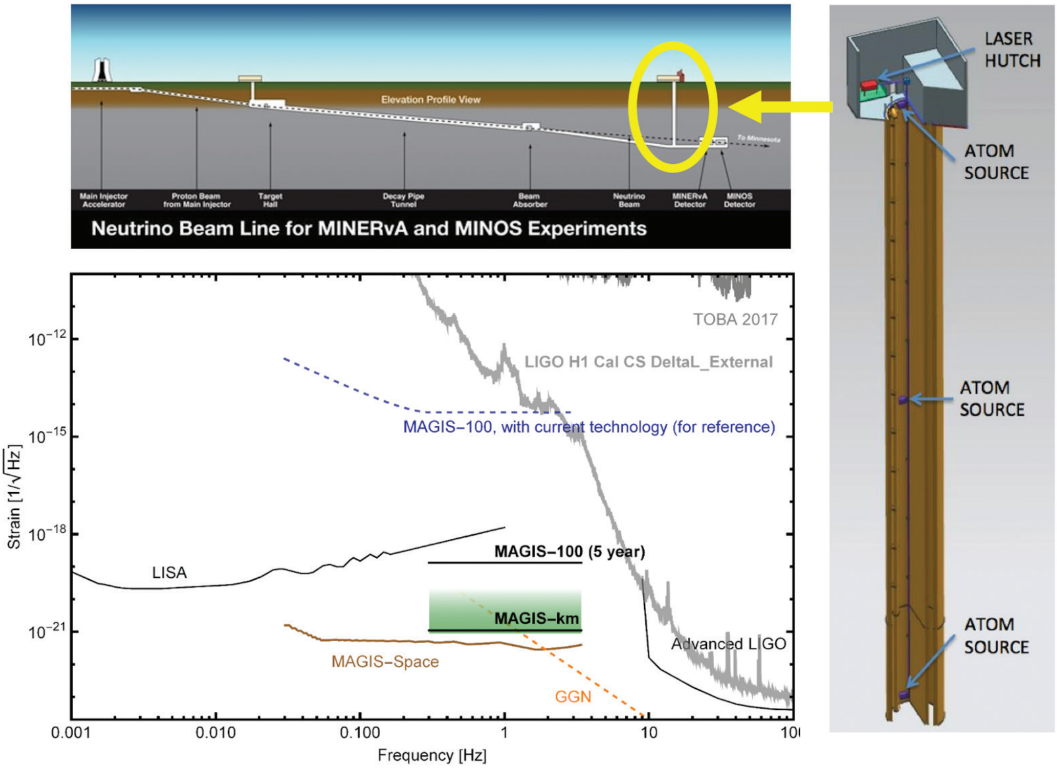

**FIGURE 6.4** *Top and right panels:* MAGIS-100 atom interferometer currently under construction at Fermilab. *Lower left panel:* Anticipated strain sensitivities of the detector as a function of gravitational wave frequency. The upper and lower atom sources are separated by 100 m. This apparatus serves as a prototype for possible space-based and longer baseline ground-based detectors (MAGIS-km). GGN indicates the anticipated level of terrestrial gravity gradient noise based on published noise models. SOURCE: Courtesy of Jason Hogan, Stanford University.

sources that include mergers of supermassive black holes, of white dwarf binaries, of neutron stars, of stellar-mass black holes, as well as supernova explosions, and yet undiscovered cosmic phenomena. As GW detectors get more sensitive, scientists can learn about the properties of these still largely mysterious sources, which in turn can increase understanding of how the universe we see came about, how stars live and die, what is the structure of neutron stars and black holes, how galaxies form, and much more.

In addition to astrophysical discoveries, GW detections also serve to teach us more about the fundamental nature of gravity, such as the speed and dispersion of GWs, the mass and spin of the graviton, whether gravitational waves permanently alter the spacetime of a region through which they have passed, and more. The precision of the measurements also makes GW detectors unique testbeds for probing the quantum limits to measurement. All in all, GW detectors use a range of AMO technologies that push the quantum limits of precision measurement to observe the dark and warped universe, while also probing the fundamental nature of gravity and quantum mechanics.

Another connection between AMO-related science and GW observations is the role of laboratory survey spectroscopy in characterizing sources. Kilonovae—the products of neutron star mergers—are predicted to be the factories in which heavy elements (with atomic number $Z \geq 44$) of the periodic table such as gold, platinum, and the actinide and lanthanide series are produced through rapid-neutron capture nucleosynthesis processes. Indeed, this appears to be borne out by optical and infrared spectra measured by telescopes in the hours following the first observation of the first merging neutron stars observed by GW detectors. To fully understand the observations, opacities are needed for low-ionization stages of heavy elements, which requires high-resolution spectral information best obtained by combining laboratory spectroscopic measurements with AMO theory. Significant advances are required in both AMO theoretical and experimental methods in order to maximize our scientific understanding of these newly discovered objects.

### Magnetometry

Measurement of magnetic fields has a long history. Work at the "precision frontier" in magnetometry not only impacts a variety of application domains but also loops back and impacts fundamental questions of physics itself. Some of the obvious areas of impact include mapping and understanding geological and geoplanetary magnetic fields, as well as magnetic fields in space both planetary and interplanetary. Other applications include the measurement of biomagnetic fields to deepen understanding in life sciences and for uses in medicine. The sensitive measurement of these fields enables noninvasive studies of the time dependence and spatial distribution of biocurrents, and has largely focused in people on the heart and brain. This includes direct field detection as well as detection of nuclear magnetic resonance (NMR) or magnetic resonance imaging (MRI) signals, for use in novel configurations such as "remote" NMR (where, e.g., the sample and the magnetometer can be spatially separated). Measurement of brain fields (magnetoencephalography) is widely used for functional brain studies—for example, localizing sensory response. Still other applications of magnetometry include detecting human-made objects, ranging from the mundane, like finding coins on a beach, to national security applications, like locating enemy tanks or submarines. In particular, for the scope of this chapter, sensitive measurement of magnetic fields plays a crucial role in the testing of fundamental symmetries. For example, magnetometers are employed in setting limits on the electron or other particle's EDM, on particular forms of violation of Lorentz invariance, and on spin-dependent forces that might be mediated by axions.

Different aspects of the measurement are important for various applications. One obvious aspect is sensitivity—namely, how small a field or difference in field is discernible. In other applications, one might perhaps trade off some sensitivity for spatial resolution. How small a domain must one be able to image? For example, macroscopic is good enough for seeing a coin or a submarine, but for these applications high sensitivity is critical so that one does not miss anything; while a neuron in a biological system, or a defect in a material requires a considerably smaller sensor head to discriminate the structure (see Figure 6.5 for the trade-off between resolution and sensitivity). Although one still desires as much sensitivity as possible, typically one gets several orders of magnitude less sensitivity in the microscopic approaches. On the other hand, one can work in a shielded environment

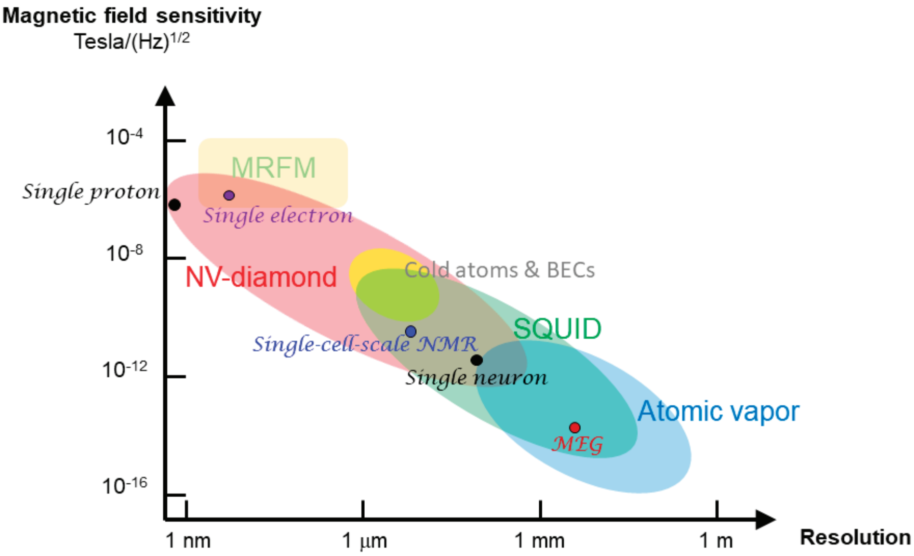

**FIGURE 6.5** This figure shows schematically, for a variety of approaches for the measurement of magnetic fields, the trade-space of two significant metrics—namely, the resolution at which one can resolve an object versus the sensitivity with which one can detect its magnetic field. The points in the diagram show the approximate required spatial resolution versus needed magnetic sensitivity in order to detect a single proton, a single electron, a biological cell by NMR, a neuron, and to do a (brain) magneto-encephalograph (MEG). The well-known Superconducting Quantum Interference Devices (SQUIDs) were long the gold standard for magnetometers, and still have important uses. However, AMO-based approaches outdo SQUIDs now, both in field sensitivity and in resolution. The different approaches shown are discussed in the text. All have additional trade-space metrics, including various needs for isolation from the environment, such as cooling, shielding from stray fields, need for operation at zero field, and the like. Magnetic Resonance Force Microscopy (MRFM) is a form of atomic force microscopy. SOURCE: Adapted from Ron Walsworth, Harvard University.

for these kinds of measurements, unlike, for example, detecting submarines in the noisy environment of Earth.

Still another trade-off is simplicity. For decades, Superconducting Quantum Interference Device (SQUID) magnetometers had been the standard for sensitivity, as they can reach close to femtotesla (1 fT = $10^{-15}$ T) level discrimination, and even provide good resolution, but they must be cooled to cryogenic temperatures. The technologies involved in cooling are generally costly, bulky, and complex. Many of the atomic magnetometers the committee discusses here do not require such cooling. Another trade-off is sensitivity versus need for shielding. A SQUID magnetometer (and others discussed) must be shielded or actively compensated to measure a small field variation superimposed on large background fields.

Magnetometers with the greatest sensitivity or spatial resolution for the types of application mentioned above are based either on SQUIDs or on AMO-related technologies. Given the added cost and complexity of cryogenic operation of SQUIDs, and that the sensitivity of AMO-based approaches is as good or better, for more and more applications the state of the art is AMO magnetometry. Figure 6.5 shows the sensitivity versus spatial resolution trade-off of various classes of magnetometers for comparison.

One of the leading classes of AMO-based magnetometers are optically pumped magnetometers (OPMs) containing thermal atoms. These can employ electron paramagnetic resonance (EPR) or NMR of atoms, generally contained in a glass vapor cell. One uses lasers to optically pump the vapor and prepare the atoms in a strongly polarized state. The gas vapor is usually of rubidium or cesium because the pumping frequencies match up very well with wavelengths available from semiconductor lasers, which can be made very small. (Helium-4 magnetometers are also widely used—for example, in space applications—because of their relative simplicity and reliability.) One then measures the Larmor precession frequency, which is proportional to the total magnetic field. This allows DC magnetic field measurements with femtotesla-level resolution. The precession frequency of the atomic spins can be monitored through the transmission of light perpendicular to the axis of precession. The precession can also be monitored through nonlinear magneto-optical rotation. Sources of loss of sensitivity are from collisions with the glass walls of the cells, and due to spin-exchange collisions with other atoms. Both can be overcome (e.g., with coatings such as paraffin on the glass walls, or going to lower densities or adding buffer gasses to reduce interparticle collisions). These steps increase the coherence time (which effectively translates to interrogation time), but do not entirely solve the problem. For example, reducing the density also reduces the overall sensitivity. Coatings, while they can be efficient, are still a "black art" and are not well understood (and thus are often not even reproducible); even ones that work very well can be thwarted with small areas of impurity. In state-of-the-art vapor cell magnetometers, very high sensitivity is achieved when decoherence due to spin-exchange collisions is suppressed—that is, by working in the spin-exchange relaxation free (SERF) regime. However, working in this regime requires working in a very low ambient magnetic field environment, very close to zero field. SERF and other zero-field OPMs can be used only in a magnetically shielded environment in which the background field is nearly zero, and the background magnetic noise is very low. A standard way to solve the problem of ambient magnetic field noise is the implementation of gradiometers, where the magnetic field in two locations is measured and subtracted. Thus, when taking all the appropriate measures, SERF and OPM magnetometers reach sensitivities lower than 1 $fT/Hz^{1/2}$.

Microscopic approaches to magnetometry are very different from the vapor cell OPM approaches. These provide much higher spatial resolution, although at the expense of sensitivity (again, see Figure 6.5). One example is related to the atomic force microscope (AFM). Such a magnetic force microscope (MFM) has reached the ability to measure the magnetic moment of a single electron. Another example of a microscopic approach uses nitrogen vacancy (NV) diamond color centers, which are described in Chapter 2. They greatly exceed the spatial resolution of OPMs and even exceed the resolution of SQUIDs. Also, unlike SQUIDs, they work well with room-temperature samples. The NV-diamonds are either embedded in the sample itself, or put at the end of a tip of an AFM. To measure magnetic field, one optically measures the effect of the Zeeman shift on the NV ground-state spin levels. However, a downside of NV-diamond vis-à-vis atomic vapor cells is that unlike atoms, NVs are in general not identical (e.g., they can occur in different lattice placements or chemical environments), and therefore a collection of NVs will typically have broadening, further contributing to lower field sensitivities. Alternatively, one may use single or small numbers of NVs, but this reduces the possible signal. Nevertheless, many exciting applications are emerging using NV-diamond, including noninvasive sensing and imaging of biomagnetism in living cells and whole animals with submicron resolution; mapping of magnetic materials within primitive meteorites and early Earth rocks with micron resolution, which is already providing advances in the understanding of the formation of the solar system and Earth's geodynamo; and imaging patterns of nanoscale magnetic fields in a wide variety of advanced materials, allowing development of smart materials.

Somewhere in between for both sensitivity and spatial resolution are trapped cold atoms and even Bose-Einstein condensates (BECs) that are created, trapped, and optically placed in close proximity to a desired target. The spatial resolution is somewhat better than with SQUIDs, but not at the NV-diamond or AFM level. Sensitivity does not reach the atomic vapor cell level, largely due to the much lower number of atoms in a BEC than in a vapor cell, despite the gain from the longer spin-coherence times. One method of detection is based on measuring density modulations—the spatially varying density measures the potential energy, which reflects the local magnetic-field. Spinor BECs are also employed, with detection based on relative populations in the different spinor states and Larmor precession among them. The most recent incarnation of a BEC-based magnetometer is the Scanning Quantum Cryogenic Atom Microscope (SQCAMscope), which is a quantum-noise-limited scanning probe magnetometer that has both high field sensitivity and micron-scale resolution. It employs a magnetically levitated atomic BEC.

One can also use cold atoms for gradient magnetometry. Two modes of operation give good results here. First, one can employ two clouds of atoms, simultaneously probing two regions of space through Raman interrogation (measuring frequency difference) to yield a magnetic field gradient. Second, one can use an atom interferometer in which one uses superposition states of two different magnetic hyperfine states that evolve differently in a magnetic field, and when recombined lead to gradient dependent fringe intensity. Cold atom-based approaches lead to sensitivities that are typically in the $\mathrm{pT/Hz^{1/2}}$ regime. From a practical point of view, however, cold atom approaches require at least a glass cell if not a vacuum chamber if one is using BECs.

In the end, the approach one uses will depend on many factors, including whether one needs high spatial resolution or high field sensitivity, the complexity of the apparatus one can deal with, including cryogenics, and whether one can work in the zero field regime or not. As described at the beginning of this Section, there are many applications of magnetometry, that range from national defense, to geology, planetary science, astrophysics, across the life sciences and medicine, to fundamental questions at the foundations of physics itself. This breadth of applications and approaches highlights the role of magnetometry as one of the AMO-based tools that enable precision measurement, both as an enabler for studies of fundamental physics and as sensors in applications in other areas of basic and applied science, and for industrial and military use. Some of these are discussed below in the context of searches for BSM physics, and others in Chapter 7 as impacts on other areas.

## THE ROLE OF THEORY AND RECENT THEORY PROGRESS

Close collaboration of theory and experiment, which is an important feature of the AMO field, is particularly important for precision measurement and fundamental physics studies. Theory has many crucial roles in these investigations, from the proposal stage to the final analysis. For example, theory is necessary to

- Develop new ideas: what other fundamental physics questions can be answered by probing atoms and molecules with precision AMO tools?
- Propose new experiments and select systems with the largest sensitivity to new physics effects of interest.

- Calculate atomic properties of the systems required for the planning and implementation of the experimental proposals and evaluation of systematic uncertainties.
- Carry out calculations needed to interpret the experiments in terms of new physics effects or set limits on possible new physics.
- Propose new tools for precision measurements—for example, to develop proposals for new clocks that are particularly sensitive to fundamental physics.

There have been exceptional advances in the accuracy of atomic and molecular structure theory in the past few years, both due to development of new methods, and to significant increases in computational resources. For example, recently developed relativistic atomic coupled-cluster codes that include single, double, and triple excitations have greatly improved accuracy for heavy atoms such as Cs, reaching 0.15-0.35 percent accuracy for transition matrix elements and hyperfine constants in this atom. Such extraordinary accuracy was required for the analysis of Cs parity violation experiments in terms of new physics as described in the section below, "Parity Violation—AMO Tests of Weak Interaction." Other advanced codes have also allowed sub-percent prediction of many properties of alkaline-earth atoms and similar systems. They are used for evaluation of blackbody radiation shifts and other systematic uncertainties in optical atomic clocks; design of highly charged ion clocks; analysis of experiments for new physics searches; creation of new state-insensitive cooling and trapping schemes for studies of degenerate quantum gases; and atom and light shift modeling used to understand and control alkaline atoms held with optical tweezers, in optical lattices for quantum simulation, and for many other applications.

Moreover, the development of several ab initio relativistic methods of increasing accuracy allows for strategies to accurately estimate uncertainties of theoretical predictions for which no experimental data are available. The development of these approaches, which include electronic correlations to a much higher degree than was previously possible, allows one to make precision theory predictions not only in alkali metal and alkaline-earth metals but in more complicated systems as well. In turn, new experiments provide benchmark results for testing the theory.

Further method developments and new code designs now in progress will allow efficient parallel computing on very large-scale computational facilities, with the goal of accurate predictions of atomic properties in even more complicated open-shell systems. Advances in molecular theory have allowed one to calculate effective electric fields with better than 10 percent accuracy in ThO and $HfF^+$; this is needed for extraction of the limits on the eEDM from experiments.

New atomic structure community codes (CI+MBPT and AMBiT) were recently documented and released for public use. Developing flexible and robust software in computational atomic and molecular physics was a topic of a 2018 National Science

Foundation (NSF)-funded workshop at the Institute for Theoretical Atomic, Molecular, and Optical Physics. The workshop identified and prioritized outstanding problems in AMO science that would benefit from a concerted community effort in developing new software tools and algorithms, leading to more rapid progress, as well as identified the best approaches and plans to address these problems.

It is worth noting that collaborations between high-energy and particle theory and AMO precision measurement research has become increasingly active and important recently. Considering the discovery potential, such collaborations should be encouraged and strengthened, for example with joint research funding.

## SEARCHES FOR NEW PHYSICS BEYOND THE STANDARD MODEL

### Searches for Permanent Electric Dipole Moments

Remarkably, table-top-scale experiments using methods of AMO physics can be sensitive to new forces and particles, similar to those sought at the largest particle colliders. Here the committee describes an important example, namely searches for a permanent EDM along the quantized spin axis of any particle. For example, an eEDM could result from a tiny deformation of the electron's charge distribution, away from perfectly spherical. AMO experiments probe such effects in both electron and nuclear sectors as described in this chapter.

An electron (and every other fundamental particle) carries with it, at all times, a tiny cloud of "virtual" particles that includes every type of particle that exists in nature, including those yet to be discovered. The cloud acts to modify the properties of the electron as seen by an observer from afar, including the shape of the charge distribution. The quantum uncertainty principle ensures that the more massive the particle, the smaller its effect on this cloud. The existence of new heavy, teraelectron volt (or trillion electron volt, TeV) energy scale particles suggested by supersymmetry and other theories, would results in EDMs within the range of current experiments.

EDMs are intrinsically linked to violations of discrete symmetries: there is an EDM only when time-reversal (T) symmetry is broken—that is, if things are different when the flow of time is reversed. This can be visualized as follows. If a particle (such as an electron) had an EDM, it would be oriented parallel or antiparallel to the particle spin. A movie of such a particle, if run backward, would be different from the original, since the spin would reverse direction while the charge distribution would remain unchanged—implying an asymmetry under T.

The SM of particle physics includes particles that carry T-violating forces, but their effect on EDMs is indirect and leads to tiny predicted values. For example, in the SM the eEDM is predicted to be about 1 billion times smaller than can currently be detected. However, it is known that nature must include new T-violating forces. Such forces are required to explain how the universe came to be made almost entirely of matter, although equal amounts of matter and antimatter would have been created in the SM description of the Big Bang. The T-violating forces in the SM are much too weak to explain the cosmologically observed imbalance between matter and antimatter. Solving this long-standing puzzle requires nature to include new, much stronger sources of T-symmetry violation.

Happily, many well-motivated extensions to the SM introduce new sources of T-violation. The new forces and new particles in these theories typically induce EDMs more directly than in the SM. Because of this, much larger EDMs often appear in these theories, although the new particles they predict are much more massive than known particles. For example, in theories where new particles have masses corresponding to energies above the TeV scale—that is, 10 times larger than the mass of the Higgs boson—the size of predicted EDMs is typically within the limits current AMO experiments could detect. Since this exceeds the scale directly accessible to current and near-future particle colliders, these AMO-based EDM experiments have a high potential for discovering new particles and forces not accessible in any other way.

AMO experiments can detect several types of T-violating effects, including EDMs of the electron, proton, and neutron, T-violating electron-nucleon and purely hadronic (nucleon-nucleon) interactions. Therefore, it is essential to conduct experiments in a variety of systems to probe for different effects. Paramagnetic systems (containing unpaired electron spins) are most sensitive to the eEDM and to one type of electron-nucleus interaction; while diamagnetic systems (with closed electron shells, but nonzero nuclear spin) are mostly sensitive to purely hadronic (nucleon-nucleon) interactions, and to other types of electron-nucleon interactions. In different theoretical models, EDMs are more likely to appear in one or the other of these systems.

In typical EDM search experiments, the particle's spins are first polarized, so their EDMs point in a known direction. Next, a strong electric field exerts a torque on the EDM, causing the spin axis to rotate. After applying this E-field for as long as possible, the final direction of the axis is measured. Last, the E-field direction is reversed, to isolate the effect due to the EDM.

A succession of experiments over decades has sought to detect an EDM in a paramagnetic system. These experiments are usually interpreted in terms of the eEDM. In the past decade, revolutionary advances in sensitivity have been made by embedding electrons inside polar molecules, where the intramolecular E-field acting on the EDM can be roughly 1,000 times larger than in other systems. The most sensitive eEDM experiment to date, known as ACME, is featured in Box 6.2.

Electron EDM results from ACME and other experiments with Tl, YbF, and $HfF^+$ molecular ions are shown in Figure 6.6. The future reach of eEDM experiments, and constraints on new physics theories, are shown. New experiments are under way or planned with ACME and with $HfF^+$, and by incorporating laser cooling and/or trapping in experiments with YbF and other molecular species.

### BOX 6.2
### The ACME Search for the Electron's Electric Dipole Moment

To search for the electron electric dipole moment (eEDM), ACME uses electrons in thorium monoxide (ThO) molecules. In addition to an extremely large intramolecular E-field, ThO has many advantageous properties. The structure of its energy levels makes it possible to easily reverse its internal E-field, not only by reversing the laboratory field that polarizes the molecules but also by preparing different internal quantum states. ThO also hold two electrons with unpaired spins: one feels a particularly large internal E-field while the other serves to cancel the magnetic moment of the first. These properties make it possible to reject many potentially large errors that could mimic the electric dipole moment (EDM) signal.

In ACME, a cryogenically cooled beam of ThO is prepared and interrogated by a suite of tunable lasers. Detection is achieved by measuring fluorescence, whose intensity depends on the angle between the final electron spin and the laser polarization. This method has yielded statistics sufficient for a factor of 100 improved sensitivity to the EDM over the past decade. While no EDM has been observed yet, ACME places an upper bound on its size at $|d_e| < 1.1 \times 10^{-29}$e cm with 90 percent confidence, where e is the elementary charge. It also sets the best limit on one type of T-violating electron-nucleon interaction. This sensitivity is sufficient to have detected the existence of particles with T-violating interactions, whose rest mass energy is as high as 3, 50, or even 100 TeV (depending on the specific theoretical model). In many cases, this far exceeds the range of particle masses that can be produced directly at CERN's Large Hadron Collider.

The scale of ACME is larger than most atomic, molecular, and optical (AMO)-based experiments, although it is still tiny compared to particle colliders: it fits in two laboratory rooms on a university campus, and is performed by a small team of faculty, students, and post-docs. This small collaboration of a dozen or so scientists has enabled unusually rapid progress in bounding the eEDM, combined with unprecedented understanding and control of possible systematic errors. A new generation of ACME is being developed, with the aim of another order of magnitude increase in sensitivity within a few years.

The atomic $^{199}$Hg EDM search is the most sensitive EDM experiment with a diamagnetic system. $^{199}$Hg has closed electron shells with zero electronic spin, but a nonzero nuclear spin $I = 1/2$; therefore, its EDM must point along the nuclear spin axis. The $^{199}$Hg experiment sets a limit on the neutron EDM, $d_n < 1.6 \times 10^{-26}$ e cm, which is more stringent by a factor of two than the best limit from direct measurements with free neutrons. It also sets the best limits on certain T-violating interactions between quarks inside the nucleus, and between electrons and the nucleus. Other experiments with diamagnetic systems have been carried out with $^{129}$Xe and $^{225}$Ra atoms, and $^{205}$TlF molecules; these provide important constraints on the multitude of underlying T-violating interactions that could lead to EDMs in diamagnetic systems. Large enhancements of the observable diamagnetic EDM signatures are found in polar molecules such as TlF or deformed nuclei such as $^{225}$Ra. Experiments based on these systems hold promise to increase the energy

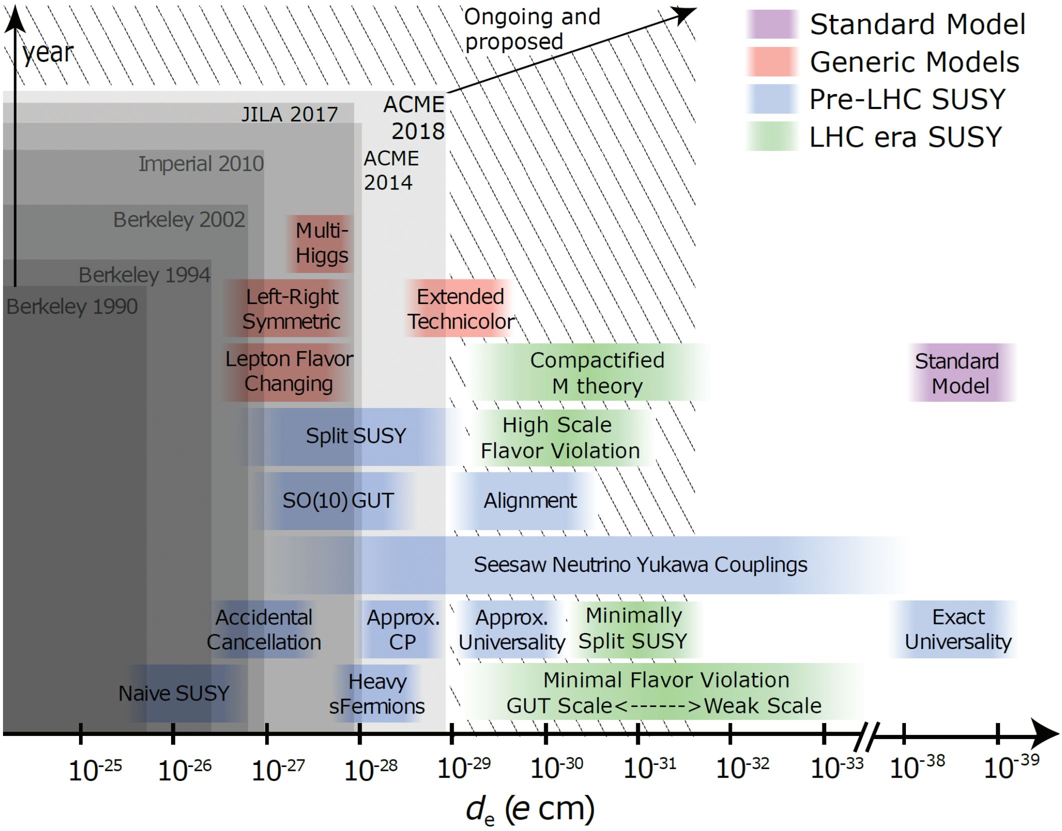

**FIGURE 6.6** Searching for new fundamental particles via the electron's electric dipole moment (eEDM). The horizontal axis shows possible values for the eEDM; gray regions show how limits have improved in the past 30 years, with the year of the experiment shown on the vertical axis. Colored regions are predictions from various theories of particle physics. The standard model of particle theory predicts a value ~9 orders of magnitude smaller than the current best bound from the ACME experiment. However, many theories that include new particles naturally predict an EDM within reach of ongoing or proposed experiments (hatched region). Note that theoretical predictions (colored regions) have evolved (green regions) in response to the absence of new particles detected at the Large Hadron Collider (LHC), direct dark matter searches, and EDM experiments. AMO-based searches for EDMs are one of the few known methods to detect evidence of new particles whose mass exceeds the reach of the LHC, within the next one to two decades. SOURCE: David DeMille, Yale University.

reach for probing new T-violating physics by an order of magnitude or more in the near future. For example, a new experiment (CeNTREX) is being constructed to improve the diamagnetic EDM limits using a cryogenic beam of TlF molecules, while $^{225}$Ra experiment is also being upgraded to further advance its sensitivity.

It is entirely plausible that EDM experiments, using AMO methods and room-scale apparatus, could provide the first new evidence for physics beyond the SM.

This would be a revolutionary discovery in particle physics, and would establish a clear benchmark for the energy needed to produce new particles in any future particle collider.

### Dark Matter, Variation of Fundamental Constants, and Fifth Force Searches

The nature of DM is one of the most outstanding puzzles in physics today. To date, experimental efforts to detect DM have largely focused on weakly interacting massive particles (WIMPs), with masses between 10 and 1,000 GeV, and has required detectors in deep underground laboratories. Despite decades of significant effort, and rapid improvements of experimental sensitivities in recent years, no conclusive signs of WIMPs have been observed. While the WIMP is theoretically well motivated, many other DM candidates inhabit a vast parameter space, all the way down to $10^{-24}$ eV, ranging from ultralight axions and axion-like particles, to more complex dark sectors that lead to composite DM "clumps."

While particle detectors work by measuring energy deposition, precision measurement techniques are well suited for detecting light mass DM candidates that act as coherent entities on the scale of individual detectors or their networks. Recent advances in optical and atom interferometry, magnetometry, and atomic clocks have stimulated a plethora of new experimental proposals for DM searches with table-top precision experiments on Earth's surface rather than underground. The key idea behind these proposals is that light DM particles have large mode occupation numbers and exhibit coherence, behaving like a wave. (DM candidates in this light mass range have to be bosonic, as the Fermi velocity exceeds the galactic escape velocity for such DM.) Many such light (below ~1eV) DM candidates have been proposed, and their effects on SM particles include the following:

1. Cause precession of nuclear and electron spins;
2. Drive currents in electromagnetic systems;
3. Induce equivalence principle-violating accelerations of matter; and
4. Modulate the values of the fundamental constants of nature, inducing changes in atomic transition frequencies and the local gravitational field.

As a result, all of the AMO precision tools discussed in this chapter—atomic clocks, interferometers, and magnetometers—can be used as DM detectors. The experiments are guided by clues from other fields of physics, suggesting mysteries that can be solved by introducing new DM candidates with particular properties. Searching for the theoretically best motivated light DM candidates gives the highest discovery potential.

SM extensions offer a plenitude of ultralight DM candidates characterized by their spin and intrinsic parity (scalar, pseudoscalar, vector, and axial vector).

The axion (pseudoscalar) is among the most well-motivated light mass DM candidates. It was introduced in quantum chromodynamics (QCD, a quantum field theory of the strong interactions between quarks, mediated by gluons) to solve the so-called strong CP problem: according to formulation of QCD the CP-violation should occur in the strong interactions but it is not observed as shown by the lack of EDMs in diamagnetic atoms and neutrons. Axions can couple to electromagnetism, can induce EDMs for nucleons via interaction with the gluon field, and can cause precession of electron and nucleon spins.

### Axion and Axion-like Particle Searches

Pseudoscalar particles such as axions and axion-like particles (ALPs) can be produced by the interaction of two photons via a process known as the Primakoff effect. This process can go in either direction, that is, in reverse an axion or ALP in a magnetic field can produce a photon (i.e., one of the two photons is supplied by the magnetic field). The ADMX experiment exploits the strong coupling of the QCD axion to the electromagnetic field in a microwave cavity, to convert axions to microwave photons in the presence of a strong magnetic field. The resonant frequency of the cavity can be tuned so that it matches the frequency of the microwave photons produced by this interaction. A new experiment, HAYSTAC, which extends the ADMX experiment to search for higher mass axions, using correspondingly higher frequency microwave cavities, has recently reported first results. Another major microwave cavity experimental program is under way in South Korea. A new broadband axion DM experiment, MADMAX, based on axion-photon conversion at the transition between different dielectric media, is under development in Germany.

A new experiment is now under way to search for lighter QCD axions and ALPs using different couplings from those exploited in ADMX/HAYSTAC, complementing these searches. The cosmic axion spin precession experiment (CASPEr) exploits both the axion-gluon coupling, which generates oscillating EDMs of nuclei (CASPEr electric), and the coupling of the axion to nuclear spins (CASPEr wind). CASPEr uses nuclear magnetic resonance (NMR) techniques for detecting spin precession caused by background axion DM. CASPEr electric has the potential to reach sensitivity to QCD axions over a five orders of magnitude in mass range (all well below ADMX), and search a significant fraction of unexplored parameter space for ALPs up to masses of $\approx 10^{-7}$ eV.

The aim of the axion resonant interaction detection experiment (ARIADNE) is to use NMR techniques to detect new interactions that can be caused by axions (see the "Fifth Force Searches" section below). The upper end of the axion mass range to be explored by ARIADNE is particularly difficult for all other DM detection experiments to access, and so ARIADNE has the potential to fill an important gap in the axion parameter space.

Spin-1 DM particles are commonly referred to as dark or hidden photons. Hidden-photon DM can be described as a weakly coupled "hidden electric field," oscillating at the hidden-photon Compton frequency (determined by its mass). It was recently proposed that both hidden photons and axion/ALPs can be searched for using tunable, resonant LC circuits. Proposals for broadband detection with LC circuits are based on the axion-photon coupling that effectively modifies Maxwell's equations—DM axions and ALPs generate an oscillating current density in the presence of a magnetic field.

In some new physics models, the initial random distribution of the scalar field in the early universe leads to the formation of domain-wall networks as the universe expands and cools. This and other mechanisms can lead to "clumpy" DM objects. The "global network of optical magnetometers to search for exotic physics" (GNOME) collaboration is searching for transient signals due to the passage of Earth through compact DM objects, such as these domain walls or DM "stars," that couple to atomic spins (similar to the ALP wind coupling searched for by CASPEr). While a single magnetometer system could detect such transient events, effective vetoing of false positive events requires an array of magnetometers.

### Variation of Fundamental Constants and Dark Matter Searches with Clocks

A fundamental constant is determined experimentally and cannot be predicted by current theories. The fine-structure constant $\alpha$, which characterizes the strength of the electromagnetic interaction between elementary particles, and the ratio of proton and electron masses $\mu = m_p/m_e$, are examples of such fundamental constants. While the very definition of the label "constants" implies that these are fixed quantities, many proposed theories beyond the SM predict that they vary in time and space. As noted above, light DM can be the source of the variation of fundamental constants. If the fundamental constants are space-time dependent, so are atomic and molecular spectra, allowing one to probe their variations from the present day to a distant past by observing light from very distance sources. Studies of quasar absorption spectra indicate that the fine-structure constant may vary on a cosmological space-time scale, but this result is controversial. The variation of the fundamental constants would also change the atomic clock tick rate, with the degree of variation depending on the atomic species of the clock. Therefore, monitoring ratios of clock frequencies over time allows one to test the constancy of fundamental constants in the laboratory. This effort has been pursued by many metrology laboratories. The combined world limits to the variation of $\alpha$ and $\mu$ are given in Figure 6.7.

The atomic clock searches initially focused on the "slow-drift" model of fundamental constant variation. Recently, it was shown that ultralight scalar DM can cause oscillatory and transient variation of fundamental constants, leading to new directions of such clock-comparison experiments. As noted above, such light mass

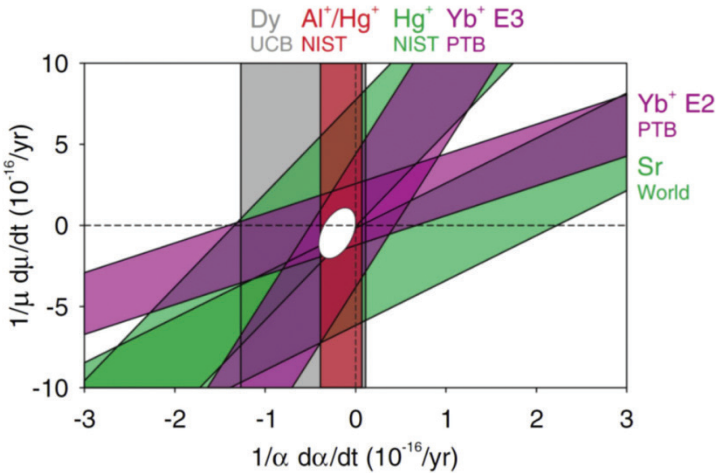

**FIGURE 6.7** Constraints on temporal variations of the fine-structure constant $\alpha$ and $\mu$ (proton-to-electron mass ratio) from comparisons of atomic transition frequencies. Filled stripes mark the 1 standard deviation $\sigma$ uncertainty regions of individual measurements, and the central blank region is bounded by the standard uncertainty ellipse resulting from the combination of all data. SOURCE: Reprinted figure with permission from N. Huntemann, B. Lipphardt, Chr. Tamm, V. Gerginov, S. Weyers, and E. Peik, Improved limit on a temporal variation of $m_p/m_e$ from comparisons of $Yb^+$ and Cs atomic clocks, *Physical Review Letters* 113:210802, 2014, https://doi.org/10.1103/PhysRevLett.113.210802; copyright 2014 by the American Physical Society.

DM permeating our galaxy exhibits coherence, behaving like a wave. Its coupling to the SM particles in atomic clocks leads to oscillations of fundamental constants and, therefore, to oscillations in clock transition frequencies, causing persistent time-varying signals that are localized in frequency determined by the DM mass. Such an oscillation signal would be detectable with atomic clocks for a large range of DM masses and interaction strengths, but would be too faint to probe with any other devices. To detect these oscillating signals, one performs measurements of ratios of clock frequencies, with minimum dead time, continuing measurements while the DM field remains coherent. Transforming the results of the time sequence measurements into the frequency domain allows one to extract the DM signal, or set limits on DM masses and interaction strengths. The first dedicated searches for such oscillating effects are ongoing in several clock laboratories.

In addition to the oscillatory changes, transient changes in fundamental constants may be induced by DM objects with large spatial extent, such as stable topological defects. Such transient signals can be observed by networks of clocks, manifesting as "glitches" propagating through the clock network. The first constraints on the coupling of such DM to SM particles was just reported with the first Earth-scale quantum sensor network based on optical atomic clocks aimed at DM detection.

### Fifth Force Searches

Presently, we know of four fundamental forces: gravity, electromagnetism, the strong nuclear force, and the weak force. These forces are characterized by their range and by their particular coupling to matter and fields. Remarkable advances in AMO measurement techniques over the past decade, coupled with new ideas emerging from theoretical particle physics, have reinvigorated AMO precision searches for forces beyond these four. For example, DM may have new interactions, whose discovery would lead to a much wider range of possible experiments for detection of the DM. An example is the ARIADNE experiment mentioned above. It is entirely possible that sufficiently feeble forces have escaped detection up to this point, and would be impossible to find with collider experiments. Startling discoveries are sometimes hiding just beyond the horizon of our measurement capability.

If a new force exists, how might it affect atoms and molecules? A way to answer this question is by quantifying all possible new forces between electrons, protons, and neutrons by "exotic physics coupling constants," establishing a common framework for interpreting different types of experiments. In this methodology, an experiment searches for a new force; if no signal is detected one establishes a constraint on one or more of the coupling constants for a length scale relevant to this experiment. In other words, experimentalists explore new regions of "coupling constant versus length scale" parameter space to determine if new forces exist, and particle theorists can interpret these results in terms of specific theories. Nearly all of the AMO community's most sophisticated experimental tools have been applied to precision searches for new forces, and have pushed the frontier of knowledge by many orders of magnitude in both coupling strength and range:

- Precision spectroscopy of atoms and molecules has constrained new atomic- and molecular-scale forces, including between matter and antimatter.
- Measurements using NV centers in diamond have constrained new forces between electrons.
- State-of-the-art atomic magnetometers have constrained a wide variety of spin-dependent forces over ranges between a cm to the radius of Earth.
- Atom interferometry has been used to search for new forces related to possible explanations of dark energy.
- Experiments with trapped and cooled atoms and ions have used quantum entanglement to constrain new forces between electrons.
- Torsion balances and cantilevers have proven to be some of the most sensitive tools with which to search both for new forces and violations of Einstein's equivalence principle.

There are a variety of exciting new experimental methods in development that promise to explore a far more extensive range of parameter space: novel NMR techniques, state-of-the-art optical atomic clocks, and opto-mechanical experiments with micron-scale objects, such as trapped and cooled microspheres and ferromagnetic needles. These all promise orders-of-magnitude improvement in sensitivity to new forces.

These are but a few examples of the wide variety of creative experiments in this vibrant field of research. Developments in the next decade offer the possibility of not only more stringent constraints on new forces, but also, perhaps, revolutionary discoveries.

### Dark Matter and New Force Searches with Future Gravitational Wave Detectors

Proposed atom interferometric GW detectors are sensitive to new physics that perturbs atomic trajectories or an atom's internal energy levels. For example, DM can lead to time-dependent signals in these detectors, enabling a unique probe of its existence. In particular, these time-dependent signals can be caused by ultralight DM candidates. Well-motivated theories indicate that the mass range from $10^{-22}$ eV to $10^{-3}$ eV is particularly interesting, and atom interferometry is a promising approach for searches at the lowest part of this mass range. Potential DM candidates within this range include the relaxions, which are particularly interesting since they appear in a recently suggested alternative solution of the hierarchy problem (via dynamical relaxation), without introducing any new physics at the TeV scale that LHC could have observed.

In addition to these DM searches, new fundamental particles may also be discovered by searching for new forces as described above. These new forces can be sourced by Earth, and if they are sufficiently long range, they may lead to differential free-fall accelerations between different elements/isotopes. A comparison between atomic sensors made out of different elements/isotopes could reveal the existence of such forces, which in MAGIS-100 can be realized by comparing two co-falling isotopes of Sr.

### Parity Violation—AMO Tests of Weak Interaction

Parity symmetry, P, changes the sign of the position vector, which corresponds to mirror reflection and 180-degree rotation. While electrodynamics is invariant under parity transformation, the weak interactions are not. At first glance, it would appear impossible to observe such a small effect in atoms, resulting from weak interactions between the atomic constituents. However, it was realized that parity violation effects are enhanced in heavy atoms as the nuclear charge cubed, leading to a series of atomic parity violation experiments in heavy atoms. Parity violation in atoms leads to a nonzero amplitude for atomic transitions otherwise forbidden by parity selection rules—for example, between the 6s and 7s states in cesium, which are of the same parity. The goals of high-precision atomic parity violation (APV) studies are to search for new physics beyond the SM by accurate determination of the "weak charge," to compare it with SM predictions, and to probe hadronic parity violation. APV is also uniquely sensitive to some DM candidates.

The analysis of a Cs APV experiment, made possible by recent advances in high-precision theory, provided the most accurate to-date test of the low-energy electroweak sector of the SM, and constrained a variety of scenarios for physics beyond the SM. Combined with the results of high-energy, large-scale collider experiments, Cs APV studies confirmed the 3 percent dependence of the electroweak force on the momentum transfer over an energy range spanning four orders of magnitude, as illustrated by Figure 6.8. The limits on extra TeV-scale Z bosons set by APV in 2009 were only recently improved upon at the LHC. APV is also uniquely sensitive to some DM models, and sets limits on a possible 50 MeV dark boson shown in Figure 6.8.

The Cs experiment was also used to probe weak hadronic interactions. This analysis yielded values of weak meson-nucleon couplings in disagreement with nuclear physics constraints, but was complicated by the difficulty of the required nuclear calculations. More experiments on other atoms or molecules are required

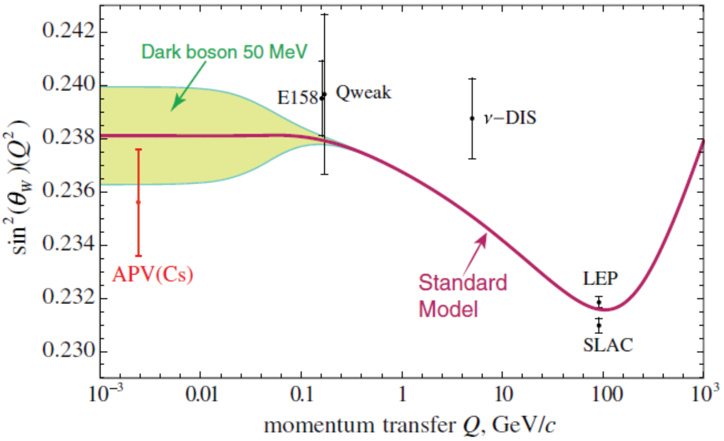

**FIGURE 6.8** Running of the weak mixing angle (quantifying the electroweak force) with momentum transfer Q. The solid red curve is the SM prediction. The table-top Cs APV result is supplemented with data from large-scale particle physics experiments whose data points are labelled. The colored area comes from one of the "new physics" scenarios: a dark boson of mass 50 MeV. SOURCE: Reprinted figure with permission from M.S. Safronova, D. Budker, D. DeMille, D.F. Jackson Kimball, A. Derevianko, and C.W. Clark, Search for new physics with atoms and molecules, *Reviews of Modern Physics* 90:025008, 2018, https://doi.org/10.1103/RevModPhys.90.025008; copyright 2018 by the American Physical Society, which was adapted from H. Davoudiasl, H.-S. Lee, and W.J. Marciano, Muon *g* – 2, rare kaon decays, and parity violation from dark bosons, *Physical Review D* 89:095006, 2014.

to solve this long-standing puzzle. Experiments with Yb (Mainz, Germany, already reported first results), Dy (also Mainz), Ra+ (Santa Barbara), Cs (Purdue), Fr (TRIUMF, Vancouver), and molecules (Yale) are currently under way.

### Testing Quantum Electrodynamics—The Most Precise Test of Any Physical Theory to Date

Quantum electrodynamics (QED) is a quantum field theory that describes electromagnetic interactions. Precision tests of QED are carried out by comparing experimental results with theoretical predictions, with truly exceptional precision reached by both theory and experiment. There have been numerous achievements in QED tests of free particle properties such as the anomalous magnetic moment of the electron, and of bound-state QED properties such as the Lamb shift. The bound tests encompass a wide variety of simple atoms and molecules, molecular ions, highly charged ions, and exotic atoms such as positronium, antiprotonic He, and so on. Only a few examples are highlighted.

### Measurement of the Fine-Structure Constant

The fine-structure constant $\alpha$, which determines the strength of the electromagnetic interaction between elementary particles, enters as an expansion parameter in QED. At present, there are two extremely accurate determinations of $\alpha$. One measurement involves determination of the electron magnetic-moment anomaly $a_e$ (i.e., deviation from the *free-electron Dirac* equation value of $a_e = 0$) carried out with a single electron that was suspended for months at a time in a cylindrical Penning trap. The ratio of electron spin-flip frequency to the cyclotron frequency in the trap determines $a_e$. The resulting value of $\alpha$, obtained by combining the experimental results with theoretical calculations including QED to the fifth order (involving >10,000 Feynman diagrams), with muonic and hadronic effects, is $\alpha = 1/137.035\,999\,084(51)$ at $3.7 \times 10^{-10}$ accuracy.

Using a completely different method, the value of $\alpha$ is also obtained from a precision measurement of the ratio of the Planck constant $h$ to the mass of an atom $M$ using atoms in a matter-wave interferometer, measuring the recoil kinetic energy transferred to or from an atom after scattering a photon. The most precise such experiment was carried out with a cloud of Cs atoms, yielding $\alpha = 1/137.035\,999\,046(27)$ at $2.0 \times 10^{-10}$ accuracy. This value does not depend on QED calculations, and the agreement between the two experiments both validates the theoretical QED calculation of $a_e$ in terms of $\alpha$ and provides the most accurate test of quantum electrodynamics (and any physical theory) to date. Work to improve both of the experiments by an order of magnitude is under way. These measurements can also be used to probe a possible substructure within the electron, and search for potential new DM particles.

## The Proton Radius Puzzle

The root mean square (r.m.s.) charge radius of the proton can be extracted from the atomic hydrogen spectrum, with the help of QED calculations, and from electron scattering experiments. A different type of experiment, using the spectroscopy measurement of muonic hydrogen (which has the atom's electron replaced by the 207 times heavier muon) was intended to improve upon these measurements. Instead, it led to the proton radius puzzle: the highly precise $r_p = 0.84087(39)$ fm extracted from the 2S-2P Lamb shift in muonic hydrogen is in significant disagreement with the result $r_p = 0.8758(77)$ fm deduced from spectroscopy with ordinary hydrogen and the electron scattering experiments. This discrepancy has prompted speculations that it may hint at new physics. Two further hydrogen spectroscopy measurements that were intended to unravel this mystery exacerbated it further, one yielding the proton radius value in agreement with the muonic hydrogen result and another supporting the previous hydrogen results. More measurements are in progress to resolve this perplexing puzzle.

## Precision Tests of Fundamental Interactions and Determination of Fundamental Constants Using Highly Charged Ions

The comparison of experimental measurements with SM theory calculations for the magnetic moment or g-factor of the bound electron in hydrogen-like ions allows further tests of QED. In this vein, the most accurate value of the electron mass, with a relative precision at the $10^{-11}$ level, is obtained by a comparison of state-of-the-art bound-state QED calculations and precise measurements of the g-factor of the single bound electron in a trapped $^{12}C^{5+}$ ion, done at Mainz (see Figure 6.9).

Highly charged ions allow to test bound-state QED in the strong-field regime ($Z\alpha$ close to unity, with Z being the nuclear charge), explored by X-ray spectroscopy for Lamb-shift measurements, by laser spectroscopy for hyperfine and fine structure, and by microwave spectroscopy of magnetic substates for bound-electron g-factor determinations. These experiments are carried out by removing most of the electrons from a heavy atom to achieve a strong-field regime. A careful comparison of results from ions in different charge states would allow for disentangling nuclear structure and QED effects to a high degree. The highest accuracy is reached with cooled highly charged ions stored in precision traps from electron-beam ion trap (EBIT) sources, or from accelerator facilities such as the ESR heavy ion storage ring at the GSI accelerator facility in Germany.

There is a competitive new experimental effort to measure the fine-structure constant as well as nuclear and isotopic effects, based on extracting heavy highly charged ions up to hydrogen-like lead $^{208}Pb^{81+}$ from the EBIT and injecting them

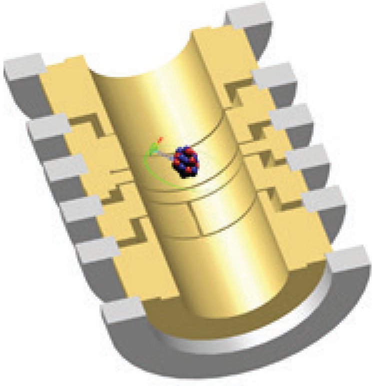

**FIGURE 6.9** A simplified sketch of a highly charged ion in a Penning trap (cut-away view). A determination of the magnetic moment (g-factor) of the bound electron allows for stringent tests of quantum electrodynamics in strong fields, as well as for the determination of fundamental constants like the mass of the electron or the fine-structure constant $\alpha$. SOURCE: Courtesy of Sven Sturm.

into the ALPHATRAP Penning-trap setup. This way, unique measurements become feasible, such as the determination of the isotopic effect in heavy highly charged ions, which gives direct and unobstructed access to nuclear effects, as well as the measurement of specifically weighted g-factor differences of hydrogen- and lithium-like heavy HCI. The latter allows cancelling nuclear effects and testing QED to high precision, as well as further pinning down of the fine-structure constant. We note the need to develop competitive HCI experiments in the United States, with many opportunities provided by new developments in the control of HCIs.

## Tests of CPT and Lorentz Symmetry

### *Tests of CPT*

Current laws of physics are believed to be invariant under CPT (the combined charge-parity-time) inversion, but symmetry breaking may arise in physics beyond the SM, such as in string theories. CPT invariance ensures the same magnetic moments and masses of particles and their corresponding antiparticles; comparisons of particle/antiparticle properties tests CPT symmetry. There has been recent breakthrough progress in these tests: The ALPHA experiment at CERN performed a laser-spectroscopic measurement of the 1S-2S transition frequency of antihydrogen, which was a long-standing goal of the antihydrogen experiments. Comparison of this result with the 1S-2S frequency in ordinary hydrogen provided a test of

CPT invariance at a relative precision of $2 \times 10^{-10}$. An observation of the hyperfine spectrum of antihydrogen was also reported.

The Baryon-Antibaryon Symmetry Experiment (BASE) reported exceptionally precise, part per billion, comparisons of antiproton and proton magnetic moments, with single trapped particles, using an advanced cryogenic multi-Penning trap system. In the future, the BASE collaboration proposes to use quantum-logic techniques to further advance CPT tests, by sympathetically cooling and probing the (anti)proton using a coupling to an atomic "qubit" ion trapped in its vicinity via the Coulomb interaction. This technique has the potential to enable proton and antiproton magnetic moment measurements at the parts per trillion level. The very recent CPT tests described above mark a turning point from proof-of-principle experiments to high-precision metrology CPT comparisons, with prospects for significant improvements in the near future.

### *Tests of Lorentz Symmetry*

Local Lorentz invariance (LLI) is a cornerstone of modern physics. It tells us that the outcome of any local nongravitational experiment is independent of the orientation and the velocity of the (freely falling) apparatus. AMO experiments may be interpreted as Lorentz-invariance tests for the photon, electron, proton, and neutron, and their combinations, with photon contributions appearing in all atomic experiments. Atomic LLI Violation (LV) experiments in the electron-photon sector exploit the different sensitivity of various energy levels to the hypothetical Lorentz violation. The quantization axis is set by the direction of the magnetic field, and the energy difference of two atomic levels with different LV sensitivities is monitored during Earth's rotation and motion around the Sun. In 2015, an experiment with $^{40}Ca^+$ trapped ions demonstrated the use of quantum information techniques (a decoherence-free subspace of a two-ion superposition) to minimize the noise due to magnetic field fluctuations, improving previous limits by a factor of 100 (see Figure 6.10).

In 2018, an experiment with two ytterbium (Yb) ion clocks improved that result by another factor of 100. Once again, precision measurement tools, specifically quantum-information-based sensors, demonstrate the remarkable potential to test fundamental physics postulates. The best tests of LLI for nucleons or photons were carried out with Cs clocks, atomic magnetometers, and rotating optical and microwave resonators.

## FUNDAMENTAL CONSTANTS AND MEASUREMENT STANDARDS

AMO methods feature centrally in defining with the greatest precision possible quantities that are of enormous technical and economic importance, such as units of distance (the meter), time (the second), and mass (the kilogram).

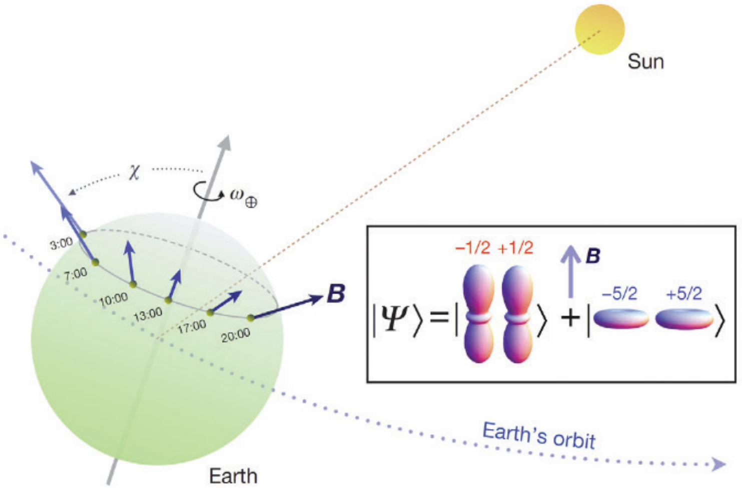

**FIGURE 6.10** $^{40}Ca^+$ LV experiment. As Earth rotates, the orientation of the magnetic field and, consequently, that of the electron wave packet (as shown in the inset in terms of probability envelopes) changes with respect to the Sun's rest frame. The states of the superposition are affected differently by the potential LLI violation, resulting in phase evolution of the wave packet with Earth rotation. SOURCE: Reprinted by permission from Springer Nature: T. Pruttivarasin, M. Ramm, S.G. Porsev, I.I. Tupitsyn, M.S. Safronova, M.A. Hohensee, and H. Häffner, Michelson–Morley analogue for electrons using trapped ions to test Lorentz symmetry, *Nature* 517:592-595, 2015, https://doi.org/10.1038/nature14091.

On November 16, 2018, the 26th meeting of the General Conference of Weights and Measures consisting of 59 member states unanimously voted to redefine the International System of Units (SI) to be based on exactly defined values of fundamental constants and invariants of nature as described in Box 6.3. The new SI officially went into effect on World Metrology Day, May 20, 2019, which means that now anyone, anywhere can realize the SI units in terms of these values combined with appropriate measurements and equations derived from the laws of nature as we presently understand them.

## SUMMARY, DISCOVERY POTENTIAL, AND GRAND CHALLENGES

### Summary

The past decade brought forth a plethora of new table-top AMO experiments aimed at discovery of new physics. While this field existed in the past, the scale of the effort and discovery potential increased so dramatically that it is considered a new emergent interdisciplinary field. This progress is expected to accelerate in

## BOX 6.3
## The Redefinition of the SI Units

The redefinition of the SI units was made possible through the ability to relate two independent experimental methods at the required accuracy and consistency; these are combined in the new SI to realize the kilogram. One method uses the determination of the Planck constant via a Kibble balance (see Figure 6.3.1), and the other uses the determination of the Avogadro constant via the X-ray crystal density method. The required comparison of these totally different methods was achievable only through the improved experimental tools and techniques of atomic, molecular, and optical (AMO) physics that enable the precise determination of the fine-structure constant, the Rydberg constant, and the mass of the electron. For example, improvements in atomic recoil measurements using Raman transitions and Bloch oscillations in optical lattices, Penning trapping techniques, quantum jump spectroscopy, quantum nondemolition coupling measurements, and higher order calculations of QED theory have led to a reduction of the fine-structure constant uncertainty by two orders of magnitude over the past 30 years. Today, these and other newly developed techniques, and the more accurate values of the fundamental constants provided by the new SI, are being used to further advance our understanding of the physical world. This includes the investigation of inconsistent results, such as the proton radius puzzle and the determination of the muon magnetic anomaly.

**FIGURE 6.3.1** The NIST-4 Kibble balance, where the weight of a test mass is offset by a force produced when an electrical current is run through a coil of wire immersed in a surrounding magnetic field. As of May 20, 2019, it uses the defining fundamental constants that form the foundation of the International System of Units (SI) to realize the kilogram. The science team consists of, from left to right in front, Frank Seifert, David Newell, Jon Pratt, Darine Haddad, and Shisong Li. In back, Stephan Schlamminger (left) and Leon Chao (right). SOURCE: National Institute of Standards and Technology, "Watt Balance Team," https://www.nist.gov/image/wattbalancegroupapril2016-2500pxresizedjpg; courtesy of J. Lee/NIST.

the next decade, with the development of new technologies and plentiful ideas for new searches. There are several important factors leading these new developments, including the following:

1. Exceptional, by many orders of magnitude, improvement in the development of AMO tools, such as atomic clocks, matter-wave interferometers, magnetometers, cold molecules, and so on. In many cases, completely new measurement technologies have been developed—for example, development of optical (in place of microwave) clocks, nitrogen vacancy centers in diamond for magnetic field measurements, atomic interferometers for many types of precision measurements, gravitational wave detectors, and so on.
2. Advances in quantum information and related technologies led to improved control of quantum systems, and enabled techniques to protect from some kinds of measurement noise, allowing one to measure at or beyond the standard quantum noise limit.
3. Significant AMO theory advances now allow rapid predictions of systems with the highest sensitivity to perform the most sensitive new physics searches, and to analyze these experiments. The theory also predicts the unknown properties needed for detailed experimental proposals, allowing one to save years of experimental work.
4. Rapid progress of dedicated AMO precision experiments—for example ACME—improved eEDM limits by two orders of magnitude, probing new physics at 3-30 TeV. This is beyond the LHC's reach. Many orders of magnitude improvement were recently demonstrated in many other new physics searches described in this chapter, including DM searches.
5. The absence of new BSM particles being discovered at the LHC strongly restricted the parameter space of supersymmetry and other theories that expect TeV scale physics. These theories had been exceptionally promising since they provided solutions to several outstanding problems: new sources of CP violation, DM candidates, and solving the hierarchy problem. Similarly, the large-scale detectors for Weakly Interacting Massive Particles (WIMPs) failed to detect them after decades of effort. With lack of experimental confirmation well within the expected mass range, the possibility that supersymmetric particles/WIMPs do not exist at the few TeV scale requires pursuing other solutions to the outstanding fundamental problems. This led to a plethora of new ideas, in particular in the area of DM searches, many of which can be realized only in AMO table-top experiments. The possibility that there is no new physics up to the 100 TeV scale is also now considered, in which case no new particles could be detected by future colliders that can be potentially built in this century. This gives increased

importance to AMO experiments probing physics at the very-high-energy scale via low-energy signals.

6. The discovery of gravitational waves from merging black holes and neutron stars using terrestrial laser interferometers has provided new opportunities for understanding the internal properties and cosmic populations of these objects. The potential for discovering new, unknown gravitational wave sources, and ultimately mapping out the gravitational wave sky over many wavelengths, is driving the design of novel next-generation gravitational wave detectors that include laser interferometers as well as atomic sensors. It is also possible that violations of general relativity may be discovered from these gravitational wave sources, possibly providing insights into a quantum theory of gravity.

## Discovery Potential

AMO searches for new physics can probe physics not accessible by colliders and other high-energy technologies. For example, search for EDMs can potentially probe physics at the 100 TeV scale, well beyond the collider-accessible energy range. Searches for violation of Lorentz invariance, CPT violation, and so on, probe physics at much higher scales. Light mass (below 1 eV) DM candidates have to be probed at low energies. The committee strongly emphasizes that most AMO experiments are table-top, and are by far less expensive than conventional high-energy searches, leading to an abundance of new physics ideas that can be explored at the same time. Considering the discovery potential of these AMO experiments, they provide a highly competitive and cost-effective pathway toward the discovery of new physics.

## Grand Challenges

1. Development of new measurement approaches and tools in the framework of quantum information science, specifically aimed at new physics searches in the other grand challenges.
2. Discovery of EDMs, or definitive ruling out of EDMs, at the levels predicted by new physics theories. This would be a revolutionary discovery in particle physics, and would establish a clear benchmark for the energy needed to produce new particles in any future particle collider.
3. Detection of DM. Fully utilize the capability of precision AMO experiments (clocks, interferometers, magnetometers, and other AMO tools) to directly detect DM or corresponding new force signals. One specific goal is to either detect or rule out the QCD axion in the entire allowable mass range.

4. Detection of new physics signals arising from a much higher energy scale, one not accessible by foreseeable future colliders. Pursue order-of-magnitude improvements in searches for variation of fundamental constants, violations of Lorentz symmetry, of the equivalence principle, of CPT invariance, and other such tests, as well as provide much improved tests of QED.
5. Develop advanced technologies for laser interferometer gravitational wave detectors that have the sensitivity to map out the visible universe. At the same time, demonstrate promising alternative technologies for the use of atomic sensors to probe gravitational physics, including proof-of-principle large-scale systems for gravitational wave detection.

## FINDINGS AND RECOMMENDATIONS

**Finding:** Rapid advances in the precision and capabilities of AMO technologies have dramatically increased the potential of AMO-based techniques to discover new physics beyond the Standard Model. The present lack of a federal funding program dedicated specifically to supporting such research at the intersection of high-energy physics and AMO is a limiting factor in fully utilizing the plethora of opportunities for new discoveries.

**Finding:** Supporting and promoting much stronger joint efforts between AMO physics, particle physics, gravitational physics, astrophysics, and cosmology is necessary to promote creative ideas and new opportunities for grand challenge discoveries with AMO-based science.

**Finding:** The United States is falling behind in deploying a diverse set of AMO precision measurement platforms and integrating tools into dedicated devices to maximize discovery potential.

**Finding:** International collaborations are needed for full realization of AMO-based science discovery potential.

**Key Recommendation: The Department of Energy's High-Energy Physics, Nuclear Physics, and Basic Energy Sciences programs should fund research on quantum sensing and pursue beyond-the-Standard-Model fundamental physics questions through AMO science-based projects.**

**Recommendation: Federal funding agencies should modify funding structures to allow for theoretical and experimental collaborations aimed at AMO science-based searches for new physics and development of diverse**

**set of AMO precision measurement platforms including larger (more than five principal investigators) and long-term (10-year) projects.**

**Recommendation: Funding agencies should establish funding structures for continued support for collaborative efforts of atomic, molecular, and optical theory and experiment with particle physics and other fields, including joint projects, joint summer schools, dedicated annual conferences, and so on.**

**Recommendation: U.S. federal agencies should establish mechanisms to co-fund international collaborations in precision searches for new physics with other worldwide funding agencies.**

# 7

# Broader Impact of AMO Science

Atomic, molecular, and optical (AMO) science advances have had enormous influence on numerous scientific disciplines and technology development, including astronomy, astrophysics, cosmology, particle physics, condensed-matter physics, life sciences, and engineering, with strong impact to present-day industry. Often times, new research concepts and development in AMO can have surprising applications in other fields of physical sciences. At the same time, the desire for developing better tools to pursue a particular research direction can stimulate new ideas in AMO. Two recent Nobel Prizes have been awarded for AMO-driven advances that have transformed biological sciences: super-resolution fluorescence microscopy (2014, Chemistry) and optical tweezers (2018, Physics). As noted previously, the 2017 Nobel Prize in Physics for the detection of gravitational waves with the Laser Interferometer Gravitational-Wave Observatory (LIGO) is a particularly remarkable example of the intersection of AMO physics with other disciplines. In this chapter, the committee discusses a range of topics outside AMO, or right at the boundaries of AMO and other scientific disciplines, listing a number of active examples where AMO physics is having strong impact. These two-way connections make AMO one of the most central and most vibrant areas in science today.

## THE LIFE SCIENCES AND AMO

Life is organized on multiple scales, from atoms assembled into molecules such as proteins and DNA, to molecules organized into cellular substructures like organelles, to the "society" of organelles and molecules comprising a cell, to the hundreds of billions of cells making up organs and the human body as a whole. Proteins are often called nanomachines because they are nanometers in size and do critical machine-like jobs in the body, but they do so with a precision and efficiency still unmatched by human-made machines. AMO sciences have helped deepen our understanding of their function in our bodies, in normal as well as in diseased states, through advances in light sources and imaging/spectroscopy technologies, and through new ways to manipulate these components, such as with the optical tweezers mentioned at the beginning of this chapter. These newfound abilities have enabled investigation at ever higher resolution, and in situations/environments closer to native conditions.

### Protein Structure Determination Using X-ray Free-Electron Lasers

X-ray crystallography can be used to obtain atomic resolution structures of proteins, but until recently has required a high-quality crystal of the material to be examined. Crystallizing a significant amount of a material is often forbiddingly difficult. This is especially true for membrane proteins, which are important therapeutic targets. Since the early days of planning for an X-ray free-electron laser (XFEL), scientists have dreamed of the possibility of making structure determinations without having to crystalize molecules, perhaps obtaining structure from even single molecules. A major step in that direction was made in 2011. Serial femtosecond crystallography, with its intense femtosecond X rays, generated diffraction signals before radiation damage could occur, using nanocrystals that are too tiny for conventional crystallography (see Figure 7.1). Combining many such diffraction patterns obtained serially gave high-resolution structural information. By precise timing of X-ray pulses relative to a laser pulse used to trigger a photochemical reaction in a light-sensitive membrane protein, we can now record movies of their structural changes on femtosecond time scales and at atomic resolution, as they perform their function in, for example, photosynthesis and vision. In the future, serial femtosecond crystallography may be extended to the single-molecule level, altogether bypassing the need for crystallization. In addition, exciting developments may emerge when X-ray measurements that are element specific are combined with other spectroscopies such as Raman.

### Single-Molecule Measurement Technologies

X-ray crystallography typically provides only a static snapshot of many possible structures of a biological molecule. Ideally, one would like to measure structural changes in real time during the functioning of a single molecule in its native environment—that is, free in solution or inside a living cell. To relate structural changes to function, powerful single-molecule measurement technologies have

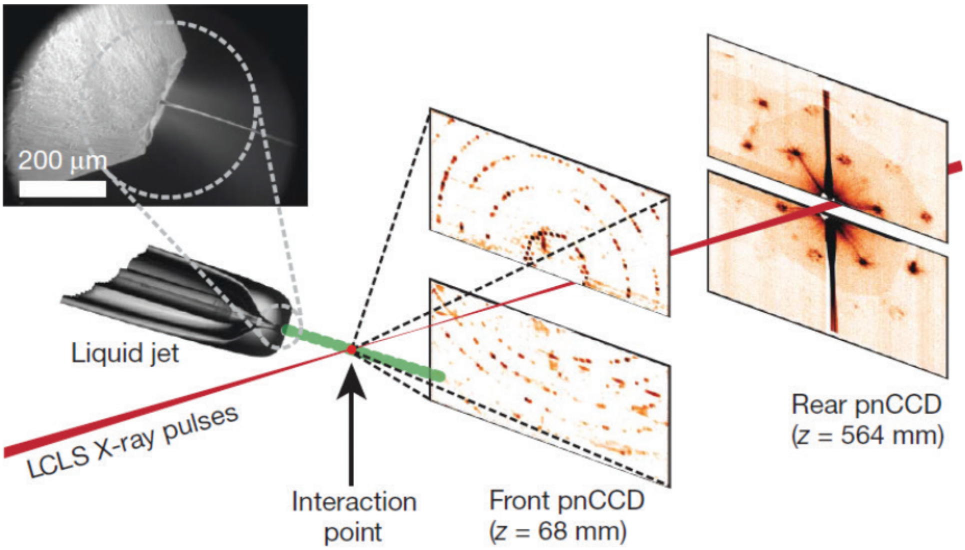

**FIGURE 7.1** Serial femtosecond crystallography using X-ray free-electron laser. Protein nanocrystals are injected through X-ray pulses shorter than the time scale of radiation damage (10-100 femtoseconds). SOURCE: From H.N. Chapman, P. Fromme, A. Barty, T.A. White, R.A. Kirian, A. Aquila, M.S. Hunter, et al., Femtosecond X-ray protein nanocrystallography, *Nature* 470:73-77, 2011, https://doi.org/10.1038/nature09750; reprinted with permission from AAAS.

been developed. For example, one can do this combining single fluorophore detection and optical tweezers (which, as mentioned earlier were respectively the subjects of the 2014 and 2018 Nobel Prizes). Optical tweezers apply pico-Newton scale forces, and detect a molecule's ~0.1 nm scale response through end-to-end distance measurements, but are blind to the intramolecular structural changes. By combining ultrahigh-resolution optical tweezer studies with single-molecule fluorescence spectroscopy, researchers are able to measure the action of a motor protein on DNA at single base pair resolution, and correlate it directly with the associated structural changes (see Figure 7.2). This hybrid single-molecule approach is just one example of maximizing the information content through simultaneous measurements of multiple observables, greatly aiding our investigation of complex biomolecular assemblages of many components.

### Super-Resolution Imaging

Super-resolution techniques have provided a new glimpse into subcellular structures, at a resolution down to 20-30 nm. This goes an order of magnitude beyond the resolution limit imposed by light diffraction, and increasingly takes us into the realm of the function of living cells. This already has had broad-based

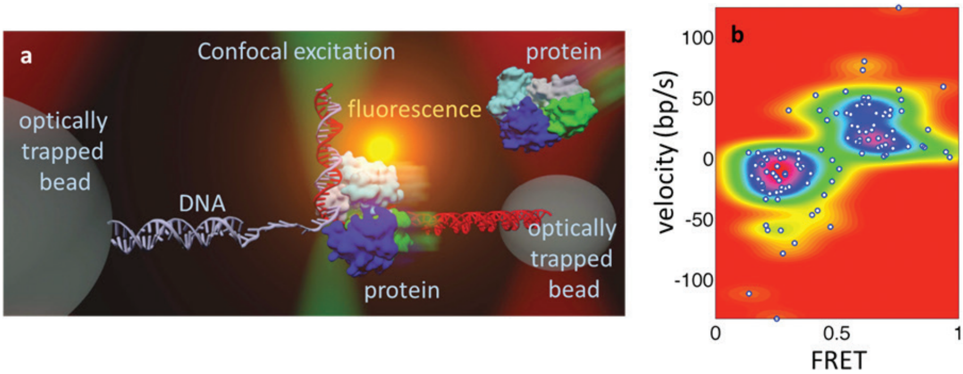

**FIGURE 7.2** Ultrahigh-resolution optical tweezers with single fluorophore sensitivity. In (a), dual optical traps apply forces to DNA segments connecting optically trapped beads, and detect DNA length changes induced by the enzymatic activity of DNA unzipping by a protein at ~0.1 nm resolution. At the same time, confocal fluorescence excitation and detection can measure the protein's structural changes. SOURCE: Matthew Comstock. In (b) one sees the correlation between DNA unzipping activity, measured by optical tweezers and expressed in reaction velocity, and protein structural changes, measured by single-molecule fluorescence resonance energy transfer (FRET) SOURCE: Comstock et al., *Science* 348:352-354, 2015.

impact not only on fundamental understanding of biological processes but also on the dysfunction that leads to disease. These advances, including stimulated emission depletion (STED) microscopy and single-molecule localization microscopy (also known through acronyms such as PALM and STORM), were recognized by the 2014 Nobel Prize in Chemistry. A striking example of biological findings uniquely enabled by super-resolution imaging is the discovery of periodic actin ring structures in neurons. (See Box 7.1, which also illustrates the concept of STORM.) In the future, super-resolution techniques will provide key insights into disease mechanisms, and we will fully visualize and characterize the "inner life of a cell" through three-dimensional (3D) imaging with true molecular resolution. All that is needed is another factor of 10 jump in spatial resolution, to about 2-3 nm. Technologies that require many fewer photons for high-resolution imaging—for example, the recently demonstrated nanometer resolution achieved with minimal photon fluxes—are promising avenues to pursue. Breakthroughs in super-resolution imaging technologies have also inspired other advances in probe development, sample preparation, and image analysis algorithms.

### Live Imaging of Native Cells and Tissues

In order to observe molecular movements and activities in their native environment, we need to be able to label individual molecules, and image them in live cells and tissues with minimal perturbation. A challenge lies in photo-toxicity. Laser excitation

## BOX 7.1
## Super-Resolution Imaging by Single-Molecule Localization

Light microscopy can probe life processes in three dimensions with a variety of contrast mechanisms, but the diffraction of light limits its spatial resolution to about half the wavelength. For fluorescence imaging, the diffraction-limited resolution is about 200 nm. An improvement in resolution up to about an order of magnitude can be obtained using super-resolution microscopy based on single-molecule localization (see Figure 7.1.1a). Imagine two single fluorescent molecules in the sample that are closer to each other than 200 nm—for example, 80 nm. If they are imaged together, each would contribute a roughly a Gaussian intensity peak centered around it, and because the width of each peak is larger than the spacing between them, the two molecules cannot be resolved as individual peaks. However, if only one of them is fluorescently active, its center can be "localized" with a much higher precision than 200 nm, routinely down to 10-20 nm, by switching off the first molecule and turning on the second and, by repeating the process, the two molecules can be resolved. Extending this principle to multiple molecules that can be switched on stochastically, super-resolved molecular structures in the cell can be obtained.

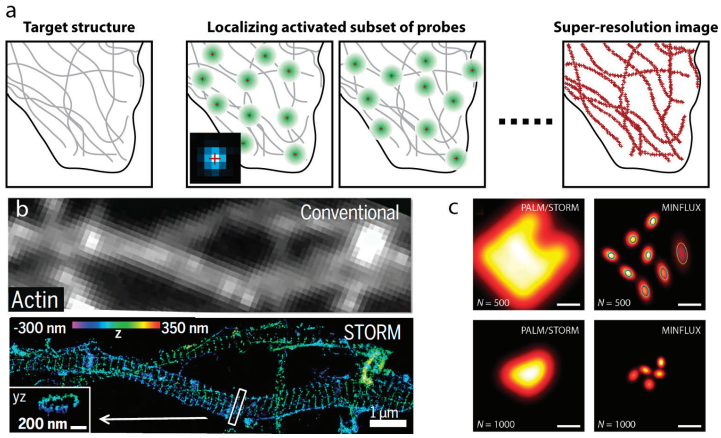

**FIGURE 7.1.1** Panel (a) shows the principle of single-molecule localization-based super-resolution imaging. Panel (b) shows an example where a super-resolution imaging method (a variation called STORM) was used to discover fundamentally new cellular structures called actin rings. By fluorescently staining actin proteins in neurons, researchers found that the actin is arranged in periodic rings around neuronal axons. Because the period is about 180 nm, conventional microscopy cannot observe such structures. Panel (c) shows a comparison of STORM images (left column) and MINFLUX images (right column) of DNA-based nanostructures. In MINFLUX, a fluorescent molecule is localized not where its intensity is maximal but where it is minimal by using a doughnut-shaped excitation spot. MINFLUX can achieve the same spatial resolution with one or two orders of magnitude fewer photons (hence its name MINFLUX). Internal structures of DNA-based nanostructures can be clearly imaged with MINFLUX (500-1,000 photons per image), whereas STORM cannot yield an image for the same number of photons. SOURCES: (a) Huang et al., *Annual Review of Biochemistry* 78:993-1016, 2009; (b) Sigal et al., *Science* 361:880-887, 2018; (c) Balzarotti et al., *Science* 355:606-612, 2017.

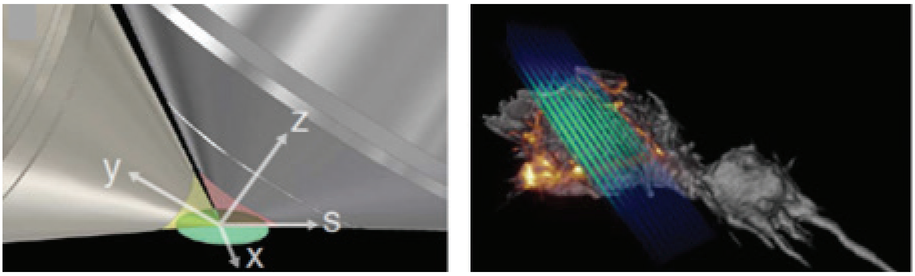

**FIGURE 7.3** Lattice light-sheet microscopy. SOURCE: Chen et al., *Science* 346:439, 2014.

of fluorescent probe molecules generates reactive oxygen species and free radicals that greatly perturb the biological processes under study, if not outright killing the cell. Light-sheet microscopy was developed to reduce phototoxicity during the imaging of large 3D samples such as tissues and whole animals. A sheet of light just 400 nm in thickness can be prepared through a special optical technique known as Bessel beam engineering, making sure that no probe is excited unless the signal is being collected from that probe. In addition to nearly eliminating phototoxicity, light-sheet microscopy greatly reduces photo-bleaching and off-focus background noise (see Figure 7.3).

It is now possible to image, at subwavelength resolution, immune cells crawling inside blood vessels in search of pathogens and tumors—even in a living animal—over hours-long time scales. Another advance is the use of adaptive optics, originally developed for astronomy, to compensate for optical aberrations that occur when light propagates through deep tissues with inhomogeneous optical properties. In addition, optogenetics has enabled newfound control over not only cellular processes (primarily neurons at this point) but also circuit-level functioning in more complex neural systems, including the brain. In the future, optogenetics will extend beyond neurons into nonexcitable cells; it will become possible to optically control the function of many different cell types, for example metabolic processes in yeast as recently demonstrated. Live cell imaging can also be performed with vibrational energy contrast, for example using stimulated Raman scattering microscopy, to probe cellular- and tissue-level dynamics with chemical specificity without the need to label the sample fluorescently. The committee expects that it may become possible to exploit quantum control effects through coherent control of light-responsive proteins to drive cell metabolism, behavior, function, and interactions.

## Medical Imaging

The way we currently examine tissues from the body under a microscope for signs of disease, known as histopathology, is archaic. Standard histopathology is moreover time and labor intensive, and in need of technological advances that will enable point-of-procedure visualization of molecular-, cellular-, and tissue-level changes. Advances in low spatial coherence light sources and speckle reduction methods (see Box 7.2), and label-free optical imaging, are bringing us closer to replacing these decades-old practices in hospitals. Challenges of multiple light scattering in deep tissue imaging may be overcome through coherent control of the light wave front. In the future, slide-free and stain-free optical imaging will first augment but then potentially replace histopathology for more point-of-care and point-of procedure medical decision making.

### Impact of Nontraditional Research Entities on AMO in Life Sciences

Instead of providing research grants, philanthropic organizations have built their own research entities. Examples are the Janelia Research Campus (JRC) by the Howard Hughes Medical Institute, the Allen Institute, and the Chan-Zuckerberg Initiative. All three have strong emphasis on developing imaging technologies. Their successes—for example, super-resolution fluorescence imaging and lattice light-sheet microscopy highlighted above and pioneered at JRC—showed that nontraditional research entities outside universities and national laboratories can nevertheless become hotbeds of innovation and discoveries. Stable institutional support for technical staff, freedom from administration and grant writing for the group leaders, and small group size may have contributed to their success. In addition, non-AMO advances—for example, the development of fluorescent probes and reporters—are motivated by advances in AMO technologies and vice versa, and such virtuous cycles can be repeated by co-localization of scientists and engineers of different breeds. More rapid adoption of the latest AMO technologies into life sciences will also become possible by raising the awareness and availability of these technologies through such co-localization.

## ASTRONOMY, ASTROPHYSICS, GRAVITATION, COSMOLOGY, AND AMO

Humanity's hunger for understanding the unknown has stimulated exciting improvements in telescopic capabilities, such as photon collection area, spatial resolution, and spectral sensitivity. AMO physics has been crucial in extracting much of what we have learned from such observations of cosmic phenomena. But while tremendous advances have resulted from these billion-dollar investments and the resulting observations, opportunities exist to learn far more by advancing our understanding of the basic underlying theory. This includes continuing to develop understanding of collisions, reactivity, and spectroscopy involving key species—for example, from applying existing methods to more astrophysically relevant molecules, to aid the simple but critical task of identifying the species being observed astronomically. Other information can be gleaned only through

## BOX 7.2
## Speckle-Reduction Using Light Manipulation and Low Spatial Coherence Light Sources

Lasers have enabled major scientific and technological advancements because of their high brightness and monochromaticity, which requires high coherence. However, high coherence can cause deleterious effects such as speckle noise, limiting laser applications in full-field imaging, parallel projection and display, materials processing, optical trapping, holography, and lithography. An example is Optical Coherence Tomography (OCT). OCT is a biomedical imaging method that uses the coherent detection of backscattered laser light to obtain morphological images of tissues. OCT is now the gold standard for diagnosis of glaucoma and a few other eye diseases and is used on millions of patients worldwide. Because of the coherence of the laser source and its detection mechanism, OCT suffers from speckle noise (see Figure 7.2.1a). By creating a large number of unrelated speckle patterns and averaging over them, we can now greatly reduce speckle noise without losing spatial resolution (see Figure 7.2.1b).

Another method to eliminate coherent artifacts in images is to use unconventional lasers with a reduced degree of spatial coherence. An example is the random laser (see Figure 7.2.2a,b). Such sources enable ultrahigh-speed massive-parallel confocal microscopy for in vivo quantitative microscale physiology. Furthermore, novel techniques have been developed for switching the spatial coherence of a laser from low to high. This allows a single source to be used in distinct microscopy modalities to obtain both structural and functional information. One

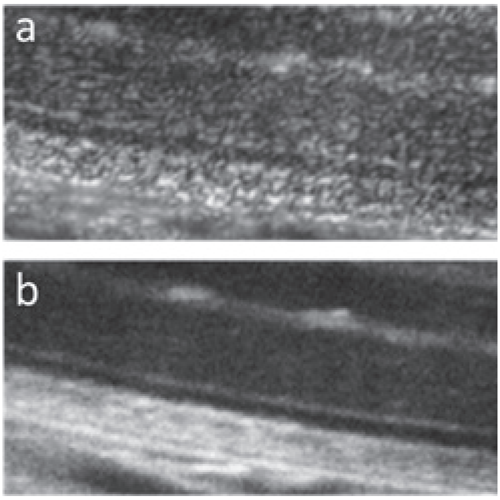

**FIGURE 7.2.1** Speckle-reduction using light manipulation. In (a) the Optical Coherence Tomography (OCT) image of a tissue specimen without light manipulation; in (b) the OCT image with light manipulation. SOURCE: O. Liba, M.D. Lew, E.D. SoRelle, R. Dutta, D. Sen, D.M. Moshfeghi, S. Chu, and A. de la Zerda, Speckle-modulating optical coherence tomography in living mice and humans, *Nature Communications* 8:15845, 2017, https://doi.org/10.1038/ncomms15845; Open Access article distributed under the terms of the Creative Commons by license.

example is dynamic multimodality biomedical imaging in living tadpole hearts, an important animal model of human heart disease. As shown in Figure 7.2.2c,d, the lower coherence illumination provides structural information, while high-coherence illumination maps blood flow in the heart because the motion of the blood cells randomizes the speckle pattern and thereby reduces the time-averaged contrast.

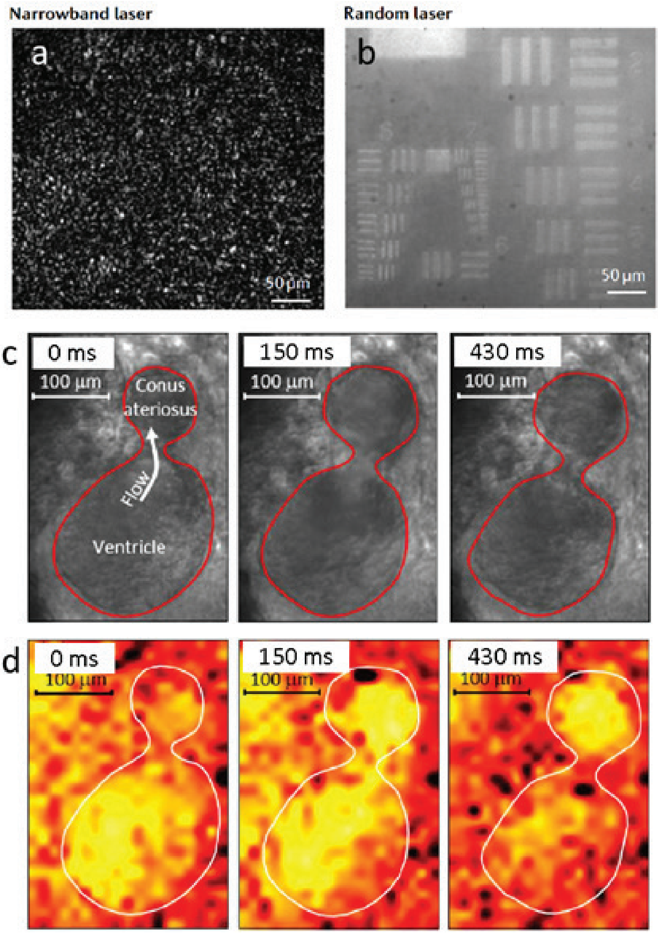

**FIGURE 7.2.2** *Panels a and b:* Speckle reduction by using random laser. *Panels c and d:* Bimodal imaging achieves speckle-reduction by using low-coherence light (c) and blood flow contrast using high-coherence light (d), in tadpole heart. SOURCE: *Panels a and b:* B. Redding, M. Choma, and H. Cao, Speckle-free laser imaging using random laser illumination, *Nature Photonics* 6:355-359, 2012, doi:10.1038/nphoton.2012.90. *Panels c and d:* S. Knitter, C. Liu, B. Redding, M.K. Khokha, M.A. Choma, and H. Cao, Coherence switching of a degenerate VECSEL for multimodality imaging, *Optica* 3:403, 2016, https://doi.org/10.1364/OPTICA.3.000403; Open Access article.

advances in fundamental theoretical understanding, computational capability, and associated advances in AMO experiments needed to describe correlated behaviors ranging from complex reactive processes, to entanglement, to AdS/CFT duality.

### Exoplanets

More than 4,000 exoplanets have been discovered to date. Observational constraints have limited these primarily to planets more massive than Earth, or with smaller separations from their host stars. Targeted searches now beginning for Earth-like planets, with masses and orbits similar to Earth's, require visible and infrared spectrometers calibrated to an accuracy of a few parts in $10^9$ or better, and with stability maintained for periods of time on the order of decades. Clues to the habitability of exoplanets are provided by their atmospheres. However, our ability to interpret exoplanetary atmospheres is limited by shortcomings in our understanding of the underlying molecular physics that generates the observed spectra.

Exoplanets circling distant stars can be discovered and their characteristics measured by two distinct methods, both involving important technologies from AMO. Direct observation of light reflected from the planet is difficult because light from the star can be of order 1 billion times more intense than the reflected planetary light. To get around this, the so-called transit method works well for the small fraction of planets (<0.5 percent for Earth-like) that happen to be perfectly aligned so that they pass in front of the star. This passage causes a partial eclipse that very slightly reduces the intensity of light from the star (by roughly 1 part in 10,000 for an Earth-like planet, leading to risks of false positives). The magnitude of the reduction can be used to measure the planet's diameter, and in the future it may ultimately be possible to detect spectral signatures of biomolecules using the stellar light that passes through the atmosphere of the planet.

The Doppler method is a complementary technique that relies on the small changes in the velocity of the star relative to Earth induced by the gravitational tug of the orbiting planet on the star. The small change in the radial velocity (RV) of the star in turn induces a very small Doppler shift in the apparent frequency of atomic spectral lines in the light emitted by the star. The RV method thus obtains the mass of the planet, and when combined with the transit method determination of the radius, one obtains the density. This is essential for determining whether the planet is rocky or gaseous. Jupiter-like giant planets can produce stellar RV oscillations of 50 m/s (see data for 51 Pegasi b;[1] and see Figure 7.4a,b), but the Sun moves only 9 cm/s due to the motion of Earth. At this low velocity, the Doppler shift of the light frequency is only 3 parts in 10 billion.

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[1] Mayor and Queloz, 1995.

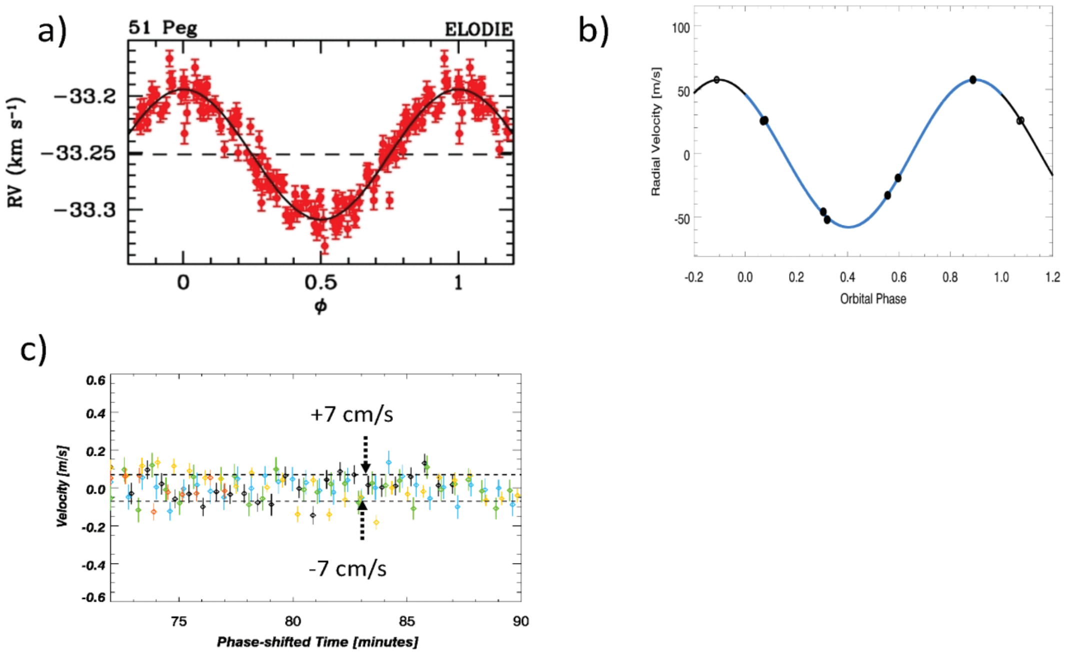

**FIGURE 7.4** (a) Original data on 51 Pegasus b showing radial velocity oscillation of the parent star of 50 m/s induced by a massive planet with short orbital period of only 4.23 days. SOURCE: M. Mayor and D. Queloz, A Jupiter-mass companion to a solar-type star, *Nature* 378:355-359, 1995. (b) Same source with current technology illustrating the dramatically reduced error bars. (c) Residuals showing radial velocity precision of 7 cm/s for the EXPRESS spectrograph. SOURCE: (a) D. Naef, M. Mayor, J.L. Beuzit, C. Perrier, D. Queloz, J.P. Sivan, and S. Udry, The ELODIE survey for northern extra-solar planets III. Three planetary candidates detected with ELODIE, *Astronomy and Astrophysics* 414(1):351-359, 2004. (b-c) Debra Fischer, Yale University.

To get a sense of just how small this Doppler shift is, the image transmitted by the spectrograph to its silicon chip CCD camera is shifted only the diameter of ~10 silicon atoms! Technological advances over the past 20 years have increased the precision of RV measurements to 7 cm/s (shown in Figure 7.4c). This remarkable feat was enabled by the AMO community's invention of optical frequency combs (astro-combs) that can lay down an array of spectral lines with fixed and stable frequency to continuously calibrate the spectrograph and remove long-term drifts due to numerous systematic errors. This is critically important because the small RV oscillations caused by Earth-like planets have to be followed for several orbital periods (i.e., several years to a decade) in order to confirm the existence of the exoplanet, and to accurately determine its orbital parameters. It has until now been essentially impossible to maintain the required level of mechanical and optical stability over multiyear periods, so the continuous absolute frequency calibration by optical frequency combs will be revolutionary for exoplanet astronomy.

AMO techniques for precision timekeeping and GPS positioning are also essential for determining the ephemeris of the telescope—the exact position and velocity changes of the telescope as Earth rotates around its axis and orbits the Sun. These effects produce huge RV changes of order 30 km/s; but through modern precision measurements these can be determined and removed from the signal with an accuracy better than 1 mm/s!

In the future, precision RV measurements of the type used to detect exoplanets will also be able to determine the accelerations of individual stars in our galactic neighborhood due to the presence of the other stars and the dark matter (DM) within our galaxy. These measurements can be used to directly probe the local gravitational potential and measure the local DM density, potentially allowing us to map out the gravitational potential of the galaxy. Knowledge of the Milky Way DM density is crucial to direct and indirect searches for the as-yet undiscovered particles comprising DM, as well as for our understanding of the standard cosmological model. Next-generation large telescopes, combined with the exquisite RV precision and stability achievable with astro-comb wavelength calibrators and exoplanet spectrographs, may make it feasible to measure stellar accelerations directly at the necessary level of $10^{-8}$ cm/s$^2$.

## The Molecular Universe

Clues to the habitability of an exoplanet can be gleaned from spectroscopic observations of the chemical composition of its atmosphere. As a planet passes before its host star, the star light is filtered by the planet's atmosphere, yielding spectroscopic data. The planned 2021 launch of the James Webb Space Telescope (JWST) will open the near- and mid-infrared (IR) range to spectroscopy of planetary atmospheres. But our ability to interpret exoplanetary atmospheres is limited by shortcomings in our understanding of the underlying molecular physics that generates the observed spectra. The spectra of many molecules are incomplete, incorrect, or completely unknown. Some of the important molecules include $H_2O$, $CO_2$, $CH_4$, $O_3$, CO, $NH_3$, TiO, VO, HCN, $C_2S_2$, $H_2S$, $PH_3$, $SO_2$, HCl, HF, OH, SiO, KOH, and KCl. Data are needed for pressure-induced line broadening parameters, continuum opacity due to collision-induced absorption, molecular opacities at high spectral resolution, photoabsorption cross-sections for molecules at high temperatures, and expanded databases for atmospherically relevant chemical reactions.

With the construction of impressive facilities such as the Atacama Large Millimeter/submillimeter Array (ALMA), the Stratospheric Observatory for Infrared Astronomy (SOFIA), and the upcoming JWST mentioned above, a flood of spectral data on complex molecular features is eagerly anticipated. However, a longstanding difficulty is the fact that the species responsible for the vast majority of the astronomically observed molecular spectral features remain unidentified. Many of these are thought to be due to complex molecules with both known and unknown spectra, such as polyaromatic hydrocarbons (PAHs), which are abundant in space. Theoretical methods are still not sufficiently accurate to predict molecular spectra reliably. Laboratory spectra are the only reliable way at present to identify molecules in space, but experimental efforts can be time consuming, and at the current rate of progress, only a few new molecules are being identified per year. The bottom line is that new AMO theoretical advances and experiments in molecular spectroscopy are needed in order to unlock the full mystery of the molecular universe. Moreover, advances in reactive scattering techniques are needed so that we can reliably model and interpret the molecular properties of the cosmos.

In some cases, application of current methods can suffice, while in many cases there are opportunities for truly creative efforts that are needed to overcome current limitations in our intellectual ability to identify even the qualitative nature of complex reaction mechanisms. One promising experimental advance is a facility that has just become operational, the ion Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg, Germany, which can measure inelastic collision rates and molecular destruction rates by electron collisions with molecular cations at the low temperatures (10-100 K) that are relevant to interstellar clouds. The Desiree Ring in Stockholm is focused on ion collisions. AMO groups in the United States also are preparing experiments to study collisions and reactions of trapped and cooled molecular ions with cold and slow beams of free radicals. At present, however, very few AMO theorists are supported in the United States to develop a theoretical interpretation of the experimental results that these facilities are beginning to produce.

## Gravity and Cosmology

As already discussed in Chapter 6, gravitational waves are opening up a new frontier in astrophysics and cosmology. Squeezed light methods, combined with enhanced power in the laser interferometer detectors, are predicted to enhance gravitational wave detection at high frequencies (50-5,000 Hz). These advances will double the spatial detection volume, provide better sky localization (source direction determination), enable better estimates for the tidal deformability parameters of the merging compact objects, open up the ability to study the post-merger phase, and constrain the neutron star equation of state. Alternative AMO ideas, such as large-scale atom-interferometric gravitational wave detectors, have the potential to open up lower frequency regimes. Continued advances in AMO techniques hold the promise of expanding our ability to use gravitational waves to help unravel the mystery of the cosmos.

In 2019, radio astronomers in the Event Horizon Telescope collaboration successfully completed a monumental 14-year quest to produce the first-ever image of a black hole 55 million light years from Earth. Resolving such a small object at such a great distance required the use of a "virtual" radio telescope effectively the size of the entire Earth—created by combining signals from many different telescopes from around the world. In order to be able to digitally combine these disparate radio signals, days and weeks after they were recorded, each one had to be "time stamped" with its exact arrival time, with exquisite resolution. This in turn required high-precision atomic clocks (commercial hydrogen masers with frequency stability of 2 parts in $10^{14}$ over 10 seconds), synchronized and given long-term stability via the GPS satellite time system, which in turn is based on rubidium atomic clocks. Without these products of AMO science, the spectacular image shown in Figure 7.5 would not have been possible.

A more foundational impact of AMO on gravitational physics (and cosmology) comes through the string-theoretic AdS/CFT duality. This is a now decades-old

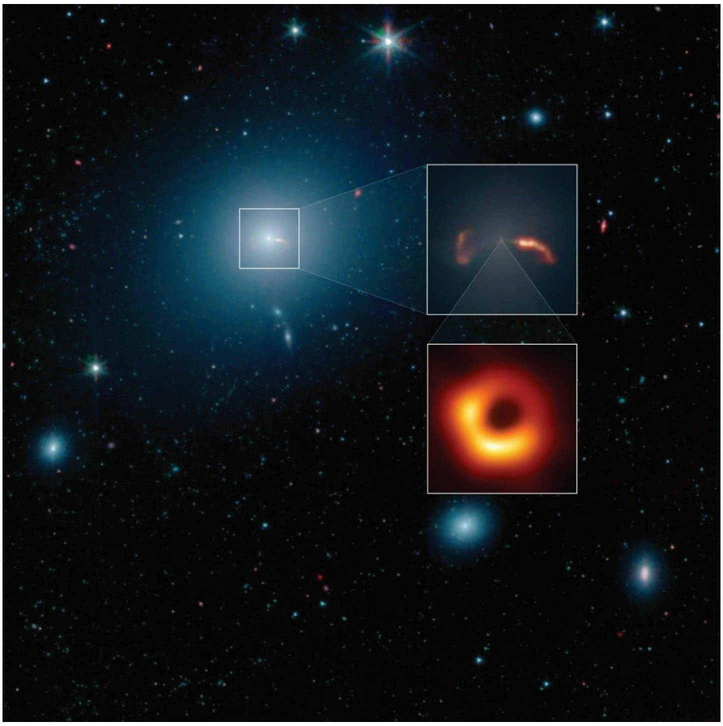

**FIGURE 7.5** NASA Spitzer Space Telescope image of the galaxy M87. Upper inset shows an infrared optical image of energetic jets of material outside the supermassive black hole. Lower inset shows the Event Horizon Telescope radio image of the black hole itself. SOURCE: NASA Jet Propulsion Laboratory, "Spitzer Captures Messier 87 (EHT)," April 25, 2019; courtesy of NASA/JPL-Caltech/IPAC/Event Horizon Telescope Collaboration.

relationship between gravitation in a particular geometric background (AdS space) and quantum theory (specifically, conformal field theory [CFT]). It has recently become clear that this AdS/CFT duality means that space-time geometry and quantum entanglement are closely related. In particular, the former could be an emergent property of the latter! In this picture, entanglement in the quantum theory is responsible for the emergence of geometry on the gravitational side of the duality. However, entanglement is also responsible for thermalization in the quantum system (see more about this in the following section). With large-scale entanglement responsible for the geometry leading to black hole formation on one side of the duality, and the process behind equilibration and thermalization (by hiding information in the inaccessible global correlations that are due to entanglement) on the other side of the duality, the "loss" of information in thermalization appears to be dual to the "black hole information paradox" of cosmology. In neither case is information really lost—it is just impossibly hard to recover.

## STATISTICAL PHYSICS, QUANTUM THERMALIZATION, EMERGENCE OF THE CLASSICAL WORLD, AND AMO

As the section title implies, AMO provides a good platform to explore how macroscopic systems are able to come to equilibrium and the emergence of the classical world from the quantum. These are possibly among the most fundamental questions in all of physics. Emergence of complexity from few-body physics is discussed in Chapter 3, along with the topic of thermalization, which has always had a bit of paradox associated with it. How can a system seemingly always move toward equilibrium when in fact the underlying dynamics is reversible due to time-reversal invariance? Chaos seemed to come to the rescue, as small perturbations could prevent the dynamics from exactly following the reverse path. But quantum mechanics throws a wrench in this picture, as there is still reversibility because of unitary evolution of the wave function. This means among other things that the entropy of the system cannot be increasing, as would be expected as one moves toward equilibrium. What then is the answer to thermalization?

Entanglement appears to be intimately connected to the answer to this and to the emergence of equilibrium, as well as of classicality. Theoretical work from the past decade or more sheds light on this by means of the eigenstate thermalization hypothesis (ETH). It is a picture that shows us how quantum systems might nevertheless thermalize. The framework in ETH that connects microscopic models and macroscopic phenomena is based on having highly entangled quantum states. As AMO provides the means to generate entangled states, it is the right field in which this hypothesis can be tested. Specifically, systems can be realized and exquisitely controlled in AMO experiments, and in quantum gas microscopes in particular. Very recent experiments employing such a quantum gas microscope studied strings of rubidium atoms confined in the wells of an optical lattice. Initially, the wells contain atoms that are isolated and noninteracting. When tunneling interactions are enabled, the system as a whole remains in a pure state, but smaller subsets of atoms start to follow a thermal distribution. This experimentally allowed the observation of the emergence of statistical mechanics in a quantum system. The fundamental role of quantum entanglement in facilitating this emergence was observed. The measurement of parts of an entangled state creates a local entropy. The subsystem is no longer a pure state, but rather in a statistically mixed state. This occurs even in as simple a system as a Bell pair of states, but occurs to a much higher degree in a strongly entangled macroscopic system.

AMO measurements in a quantum gas microscope enable such measurements, and have in fact shown that the approach to equilibrium is consistent with the ETH. A globally pure quantum state is acting at a local level like a classical system evolving under the laws of statistical mechanics.

In this understanding, thermalization in a quantum system happens despite unitarity: information is not lost but inexorably hidden in the growingly inaccessible complex global correlations resulting from entanglement, which are inaccessible to local measurements.

It is more speculative, but it appears that the entanglement entropy, the source of thermalization, might also be responsible for the emergence of the observed classicality of our experienced world. This local classicality then allows for dynamics that is (also locally) classically chaotic, taking us full circle back to how chaos indeed does help to explain thermalization after all.

In conclusion, AMO-based ideas and approaches, in particular revolving around creation and manipulation of entanglement, could be central to answering questions as significant as the emergence of the second law of thermodynamics, the emergence of gravitation, and the very emergence of the classical world. AMO science can continue to contribute to these foundational questions through studies of large-scale entanglement.

## CONDENSED MATTER AND AMO

It was not all that long ago since Art Schawlow said, jokingly, of AMO physics that "a diatomic molecule has one atom too many." Nevertheless, for two decades now atomic physics has ventured well beyond two atoms, and well beyond even molecular physics.

The impact of AMO physics on statistical mechanics and condensed-matter physics (CMP) came through the creation first of Bose-Einstein condensates (BECs), and then quantum degenerate Fermi gases, exploring their crossover, exotic pairing mechanisms, and other questions clearly in the realm of statistical mechanics. This trend is picking up speed in areas such as the creation and study of novel phases of matter (including dynamically induced phases). Unlike in CMP, the interactions in AMO physics are readily tunable, and the systems are "clean" (e.g., largely without defects or disorder unless one wishes to explicitly study those effects, and if desired, limited to only those terms considered to embody the key physics).

Over the past decade, AMO-based quantum simulation, particularly of CMP phenomena, has become ever more widespread in use and application. At the same time, techniques have been continually refined, becoming ever more controlled, having moved from simple optical lattices to quantum gas microscopes to the current degree of sublime control seen in optical tweezer arrays (highlighted in Chapters 3 and 4). In the simulated systems, one can go beyond studying novel phases of matter and phase transitions—for example, by investigation of otherwise inaccessible quantum phase transitions (occurring at zero absolute temperature). One can also study CMP model Hamiltonians that underlie a variety of phenomena including magnetism and novel superconductivity. Furthermore, AMO techniques permit direct access to the full wave function of the model system through measurement techniques not generally available in CMP.

A specific question under study this past decade, but still to be resolved, is the nature of high-temperature superconductivity. Does the Fermi-Hubbard model (an extremely elegant but highly simplified model) contain the necessary physics? And if not, what minimal additional terms might be required? Computer simulations of even this simple model are intractable because of the exponential scaling of the dimensionality of the Hilbert space with the number of quantum particles. AMO-based quantum simulation has been demonstrated on systems far larger than anything tractable on a classical computer—for example, the antiferromagnetic Néel state has been observed. However, the high-temperature superconducting phase remains elusive. Is this phase to be found in this simple model? Holding AMO-based studies back at the moment is the necessity of reaching yet colder temperatures, and more fundamentally, understanding how and under what circumstances closed quantum systems reach equilibrium (discussed in the previous section). These obstacles are themselves important and unsolved problems traditionally considered outside the realm of AMO physics—but now very much a part of it.

Additionally, AMO physics has become the realm in which to observe many CMP phenomena clearly and cleanly, such as the Mott insulator transition, Bloch oscillations (due to the presence of "tilted" periodic potentials), and perhaps soon, quantum spin liquids. The connection between CMP and AMO has been growing since the realization of BECs, with the area of quantum simulations of CMP systems as described above being a big one in recent years. A few specific examples of this growing crossover between these fields that has taken place during this past decade can be seen in the two highlights described below.

### Polariton Bose-Einstein Condensates

Excitons are an analogue for CMP of what the hydrogen atom is for atomic physics. They are hydrogen-like bound states of a negatively charged electron in the conduction band and a positively charged hole (missing electron) in the valence band of a semiconductor. When a photon travels through a solid, it can be absorbed to create an exciton. Conversely, the exciton can disappear by annihilating the electron with its antiparticle (the hole) and creating a photon. Remarkably, when these two processes are quantum coherent, the true excitation in the solid is neither photon nor exciton but a coherent superposition of both at the same time. Such coherent light-matter excitations are known as polaritons.

In the past decade, there has been exciting experimental progress in engineering the properties of excitons in artificially structured semiconductors. As shown in Figure 7.6, the excitons can be confined to a thin, two-dimensional (2D) sheet by means of a quantum well, and the photons can be confined to the same region by a pair of surrounding mirrors that are highly reflecting. This results in the formation of highly coherent polaritons with lifetimes that are greatly enhanced by the confinement.

In addition, the confinement gives the polaritons an effective mass that is three orders of magnitude smaller than the electron mass. The low mass in turn means that the particles can form a Bose-Einstein condensate, not at the 100 nano-Kelvin scale seen for cold atomic gases, but rather at temperatures of tens of Kelvins, as shown in Figure 7.7. Furthermore, unlike ordinary photons, polaritons can collide and scatter from each other due to their repulsive interactions. This means that on top of forming a BEC, they also form a superfluid that can flow past obstacles

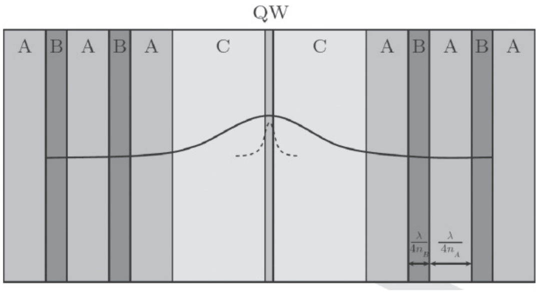

**FIGURE 7.6** Artificial structure consisting of layers of different semiconductors. The quantum well (QW) in the center has a smaller bandgap than the surrounding material, and so excitons created in the well are confined to that layer. The surrounding layers form a pair of highly reflecting mirrors (distributed Bragg reflectors) that trap photons bouncing between them. Because the photons and excitons are confined to the same two-dimensional region of space, polariton formation is strongly enhanced. SOURCE: S.M. Girvin and K. Yang, “Bose–Einstein Condensation and Superfluidity,” pp. 531-548 in *Modern Condensed-Matter Physics*, Cambridge University Press, 2019.

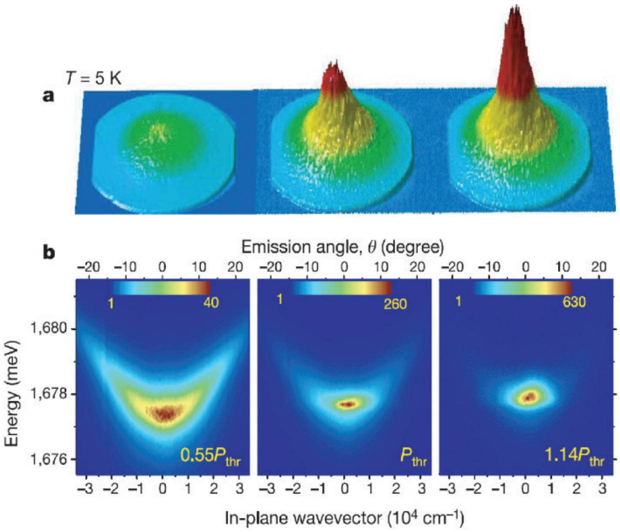

**FIGURE 7.7** Bose-Einstein condensation of polaritons in a two-dimensional (2D) quantum well at a temperature of approximately $T \sim 5$ K. The transition occurs at ~tens of K. (a) Quasi-equilibrium momentum distribution of polaritons at three different densities. The momentum vector is determined by the angle of emission of photons that slowly escape from the condensate through the Distributed Bragg Reflector (DBR) whose reflectivity is slightly less than unity. Note the remarkable similarity to observations made for a cold atom system at $T \sim 100$ nK. (b) Direct display of the polariton population at different points on the dispersion curve. The energy is determined by the frequency of photons emitted from the condensate through the DBR. The momentum is determined from the angle of emission relative to the normal to the 2D system. SOURCE: Reprinted by permission from Springer Nature: J. Kasprzak, M. Richard, S. Kundermann, A. Baas, P. Jeambrun, J.M.J. Keeling, F.M. Marchetti, et al., Bose–Einstein condensation of exciton polaritons, *Nature* 443:409-414, 2006, https://doi.org/10.1038/nature05131; copyright 2006.

without any resistance. This can be directly observed experimentally by using a tilted laser beam to form the polariton condensate with nonzero momentum that allows the experimenter for the first time to directly image the quantum wave function associated with superfluid flow around obstacles. The repulsive interactions bring in other related phenomena including collective density waves that travel through the polaritons "fluid" at what can be called the "speed of sound of light." This is one example of an exciting new subfield that is opening up in which photons and polaritons are the elementary quanta of correlated and interacting quantum systems.

## Light-Induced Phases of Matter

When an intense laser pulse is incident on a material, light is typically absorbed by the electrons, resulting in an electronic excited state. However, if the energy of the light is tuned to a frequency below the absorption threshold, novel quantum effects can come into play. In this regime, light can coherently hybridize with electrons inside the solid, generating quantum superpositions of photon-electron states named Floquet-Bloch (FB) states. Experimental observation of these states was recently achieved by making a "movie" of the electronic energy levels while the material was illuminated with low-frequency light. This discovery paves the way for optical manipulation of quantum states of matter. It could enable changing the phase of a material with light, such as switching it from being conducting to insulating, or transparent to opaque, simply by changing the properties of the light such as polarization, intensity, or frequency. For example, the symmetry that makes the energy of two different electronic states ("valleys") equal in certain semiconductors can be broken using circularly polarized light, lifting the energy degeneracy as if a huge magnetic field had been applied. In other materials, the application of light seems to enhance the appearance of superconductivity. The field of light-controlled solid matter is still in its infancy, but from these examples it seems to hold promise for the manipulation of matter, both in furthering science and for future applications.

## ADVANCED ACCELERATOR CONCEPTS

Another connection of AMO physics, this time to the high-energy frontier, is through accelerator physics. Although not a new idea, over the past decade breakthroughs in AMO science have led to laser technologies that will enable so-called wake-field accelerators that would be far more compact (and economical) than conventional large-scale particle accelerators (often kms in scale). The radiation pressure from laser pulses fired into a plasma can lead to electrostatic forces (in the laser's wake, consisting of greatly separated charges in the plasma) that are three orders of magnitude larger than can now be reached with traditional accelerators such as RF linacs. Ultimately, if current experiments in this field can be scaled, that translates to either accelerators three orders of magnitude smaller (meters rather than kms), or to three orders of magnitude higher energy phenomena that can be probed.

## INTEGRATED OPTICS AND AMO

### Dynamic Control of Programmable Nanophotonic Processors

Photonic integrated circuits (PICs) have become increasingly important in both telecommunications and interconnects for high-performance computers and data centers. As complementary metal-oxide-semiconductor (CMOS)-based central processing units (CPUs)/graphical processing units (GPUs) and von Neumann computer architectures reach their fundamental physical limits, analog computing techniques that enable nontraditional architectures have begun to show promise as hardware accelerators for otherwise intractable problems. One of the most important photonic building blocks that enable these new approaches is the chip-scale PIC that can perform analog fully parallel universal linear algebra operations on optical signals. These systems are electrically reconfigurable, and enable one to solve computationally complex emerging applications in classical information processing, such as efficient quantum transport simulations in the presence of disorder, and machine learning. For a more general-purpose optical computer, additional information processing functionality—such as nonlinear gates and storage—are still required. For example, an artificial photonic molecule with two distinct energy levels can be created by coupling two micro-ring resonators that have resonance frequencies and phases that can be precisely manipulated by a microwave source. Such a system is scalable and manufacturable, and exhibits the control of frequency, amplitude, and phase of photons needed for classical and quantum information processing. Future advances utilizing nonlinear optical effects in low-loss materials would enable all-optical control of chip-scale photonic logic and switching circuits, thereby bypassing the need for an optical transistor as a separate component. These techniques have led to proposals for all-optical accelerators, with such accelerators already appearing in the literature, that could tackle traditionally intractable computations, such as the exponentially difficult "traveling salesman problem," that is an archetypal scheduling/optimization problem that cannot in general be solved in reasonable time on current digital computers.

### Neuromorphic Computing and Communication

Machine Learning (ML)—a subdiscipline of "Artificial Intelligence"—is a 50-year-old field that has seen ebbs and flows of excitement and funding support and is currently making great strides. Unlike most modern classical and quantum information processing models, approaches to ML that are used to extract meaning from extraordinarily large data sets (from hundreds of petabytes to tens of exabytes) tend to arise from intuition rather than proof, and rely heavily on a variety of algorithms executed on not particularly intelligent computing platforms. For example, Reservoir Computing (RC) has become a promising analog approach to building neuromorphic computing technologies (which include analog circuitry intended to mimic the nervous system) that accomplish complex time-dependent ML tasks very efficiently. In RC, the reservoir is a nonlinear dynamical system comprising an arbitrarily connected network of artificial neurons. Training is performed only at the output layer by manipulating dynamical variables external to the reservoir to match the output to a desired target. Unlike approaches based on artificial neural networks, the internal dynamical variables never change once the computation has begun, greatly reducing the time to solution for problems from diverse fields such as communications, robotics, economics, and neuroscience. Recently, great progress has been made in building RC platforms using photonic components, outperforming conventional electronic reservoirs through high bandwidth and parallelism. In the future, a deeper understanding of how RC converges to a solution to an ML problem could lead to an initial understanding of the underlying behavior of more complicated approaches (such as neural networks), and could provide the practical background that would allow highly integrated implementations of these networks on photonic chips. Applying large-scale integrated photonics to engineered neuromorphic systems—based on artificial optical neurons—has already made significant progress in studies of spiking neural networks as analogues of simply connected biological brains. The inherent scalability of integrated optics, as well as the flexibility of connectivity in the optical circuits, could lead to a deeper understanding of learning and perhaps even neuroplasticity.

## AMO AND ECONOMIC OPPORTUNITIES

### Fundamental Science Pushes Industry to New Technologies

For decades, AMO has worked closely with industry to significantly improve the performance of components used in advanced experiments. An important recent example is the Laser Interferometer Gravitational-Wave Observatory (LIGO), which must measure movements of 10 kg mirrors by distances thousands of times smaller than the diameter of a proton in order to detect gravitational waves. Manufacturers of lasers, mirror substrates and coatings, and photodetectors have collaborated with LIGO scientists to build an optical system that operates with unprecedented precision. A newly industry-engineered highly stable and low-output-noise laser oscillator design provides the fundamental wavelength reference for the measurements. The commercially available fused silica test mass mirror substrates are so pure that they absorb less than one out of every 1,000,000 photons that pass through. The surface curvature of those substrates is so perfect that it varies from its design by only a few atomic layers.

### Commercial Off-the-Shelf Technology Enables New Fundamental Science

Some laboratory discoveries and inventions flowing out of fundamental research transfer to industry and result in commercial off-the-shelf technologies (COTs) that have wide applications and economic impact. Some of these technologies can then flow back into the laboratory to help produce new scientific discoveries.

One interesting example is the Dragonfly Telescope Project, which operates two clusters of 24 commercial telephoto lenses (see Figure 7.8) that in combination act as an extremely fast 1 m f/0.4 refracting telescope. The enormous commercial investment in perfecting the multiple lenses and anti-reflection coatings in each telephoto lens pays off for basic science in the diffraction-limited images across a wide field of view. A key feature of the high optical quality of this commercial technology is that the lens coatings are not smooth, but rather covered with tiny cone-like projections smaller than the wavelength of light. These cause the light to

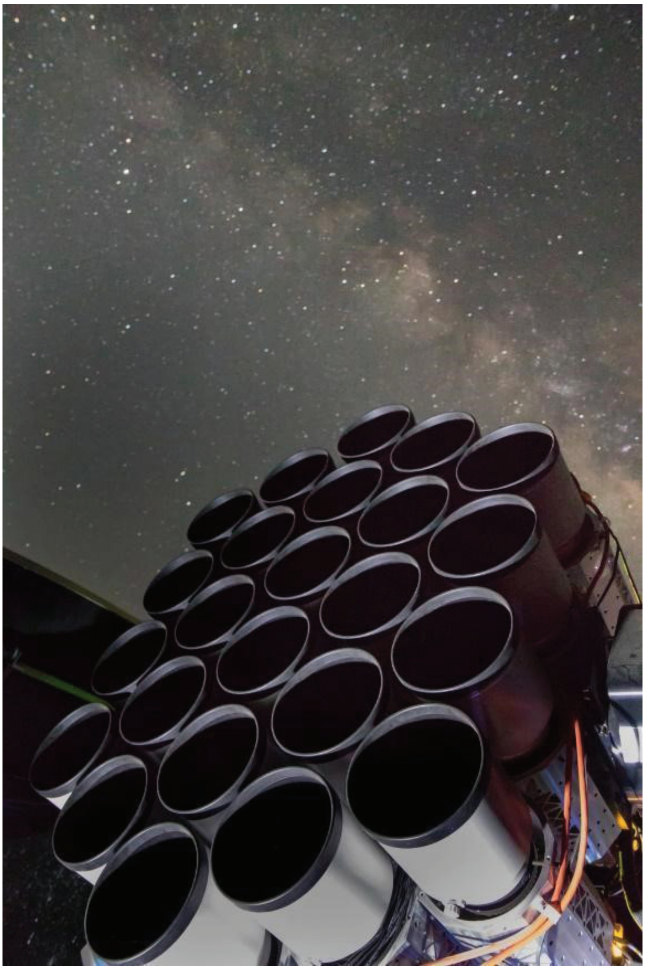

**FIGURE 7.8** One of two 24-lens dragonfly clusters of commercial 400 mm telephoto lenses. SOURCE: Courtesy of Pieter van Dokkum.

see a more gradual transition from air to glass as it enters the lens. This dramatically reduces the amount of scattered light, making the telescope ideal for imaging extended objects with very low surface brightness in the presence of bright foreground stars. This capability has led to a plethora of unexpected discoveries, including new companion galaxies surrounding the Milky Way, extremely dim galaxies that consist almost entirely of DM, and other apparently very sparse galaxies that have unexpectedly little DM (see, e.g., Figure 7.9).

Another example is the recent demonstration that it is possible to build planar ion traps in commercial complementary metal oxide semiconductor (CMOS) manufacturing facilities, which can offer improved design reproducibility, lower fabrication costs, and scalability. Standard CMOS processes, including doped active regions and metal interconnect layers, allow co-integration of CMOS digital and analog electronic circuits, as well as devices for all-optical control and detection. This approach to ion traps replaces the surface electrodes with a metal layer acting as the ground plane between a trapping layer and the underlying p-type doped silicon substrate. Incorporating the integrated photonics techniques described above, commercial CMOS technologies enable co-design and fabrication of robust and stable platforms for large-scale quantum processing in trapped ion arrays.

**FIGURE 7.9** Ghostly "see through" galaxy containing almost no dark matter discovered using the dragonfly telescope. SOURCE: Courtesy of Pieter van Dokkum.

## AMO Creates New Technologies for Business

Over the past five decades, AMO fundamental science has led to hundreds of inventions and new technologies that touch our daily lives. Some of the areas impacted include the following:

- New imaging and analysis techniques for biomedicine;
- Flat-panel TVs, computer and mobile-phone displays (now 3D);
- Cheaper, more efficient light sources;
- Solar cells;
- Enhanced navigation and communications;
- Improved national security and defense;
- Chemical, biological, and environmental sensors; and
- Power transmission.

In addition, many innovations—such as high-resolution microscopes and telescopes, and frequency combs for metrology and communication—substantially enhance our ability to do experimental science and build new commercially available disruptive technologies. Without a specific application in mind, 50 years ago, Charles Kao asked a simple question: is there a limit to how clear glass can be made? After more than a decade of work, his discoveries, based on answering that question, led to practical optical fiber telecommunications and the Internet. Similarly, in the 1980s and 1990s, researchers began exploring the use of submicron silicon-on-insulator optical structures to create a wide variety of devices and functionalities, launching the field of "silicon photonics." Many of these ideas have been adopted by industry to create high-performance alternatives to copper wiring for data communications in high-performance computers and large-scale data centers. Data centers and high-performance computers are likely to be the main consumers of optical chips, which consist of massively integrated lasers, modulators, and detectors acting as transmitters and receivers of ultrahigh bandwidth data. As shown in Figure 7.10, photonic devices and circuits can now be fabricated in standard CMOS foundries with densities and performance that exceed those of a decade ago by factors of 10 to 1,000.

The interactions between researchers and industry in large-scale integrated nanophotonics has led to a fruitful circle of research and advanced development, where improved scalable fabrication of silicon photonic components can be adopted by AMO scientists, and the discoveries provided by those scientists can in turn drive new commercial offerings. At this time, silicon photonics has not become as ubiquitous as silicon electronics, primarily because integrated optics continues to follow a "vertical" business model, where design and manufacturing are performed by each company separately. By contrast, the CMOS industry has

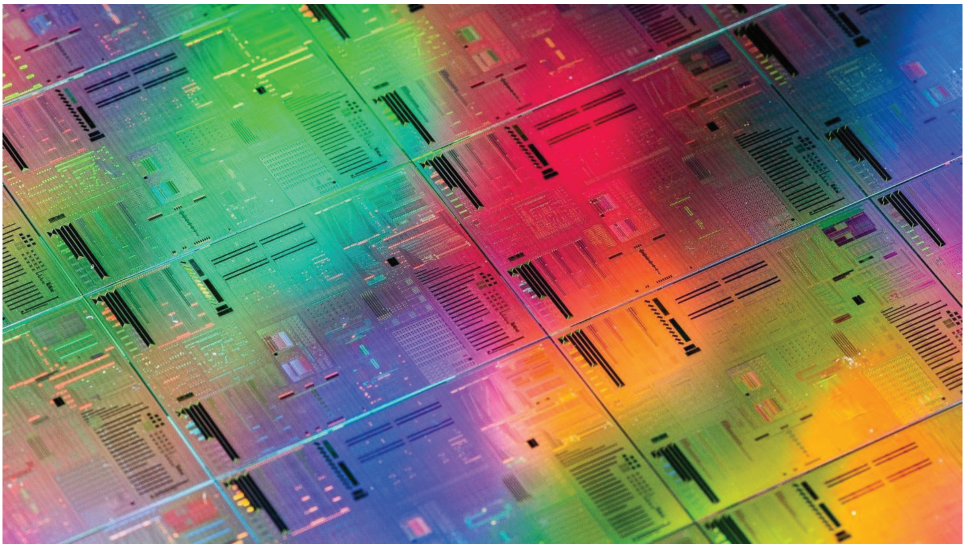

**FIGURE 7.10** Photograph of a 300 mm silicon-photonic wafer designed by Hewlett Packard Laboratories and fabricated in a 65 nm process flow, a direct result of a multi-decade collaboration between AMO scientists and engineers in academia and industry. Each die (segment) contains hundreds of nanophotonic circuits comprising thousands of integrated optical components. Testing of individual circuit elements can be performed using a standard industrial CMOS wafer measurement station augmented with fiber-optic probes. SOURCE: Rebecca Lewington, Hewlett Packard Enterprise.

adopted a "horizontal" approach that encourages design, fabrication, and packaging distributed across multiple vendors, across a broad industrial ecosystem. Democratizing integrated nanophotonics—and extending the reach and duration of the virtuous circle—by opening photonic process design kits (PDKs) to all customers at each CMOS foundry could provide a platform for the same sort of multi-project wafer runs that are the staple of electrical engineering education, research, and advanced development. These tools will represent the know-how for high-yield silicon photonic device and circuit fabrication in much the same way that current electronic PDKs provide this service for the entire electronics industry. There is a rich opportunity here to continue the creation of AMO-inspired science and engineering user facilities at universities with state government and industry-based joint support, as described next.

AMO scientific advances in the past decade have spawned a new cohort of fledgling technology companies aimed at addressing and developing markets that have been opened by those advances. The existence of many of these companies is a direct product of both global government investment in basic science at the university level and global government programs designed to transition academic innovation into commercial markets. While it is too early to assess economic impact, many of these technologies are potentially disruptive, and could lead to substantial new markets, innovation cycles, and application areas. Examples include recently formed computing companies seeking to develop quantum and photonic computing platforms; secure communication and networking companies seeking to commercialize secure quantum protocols; medical diagnostic companies based on state-of-the-art atomic vapor and solid-state defect magnetometers; precision navigation companies exploiting advances in atom interferometry and time and frequency technologies; environmental monitoring and geophysical exploration companies seeking development of next-generation geophysical and environmental sensors; and other novel sensing companies. Markets include information, communication, medical and aerospace technologies. Other companies address supply chain markets that provide innovative AMO-based building-block technologies such as lasers and photonics components to university, government, and industrial customers. These companies provide a foundation for rapid-cycle innovation by providing off-the-shelf sourcing for otherwise commercially unavailable, leading-edge tools and play a vital and central role in the research and development ecosystem.

## JOINTLY SPONSORED INTERDISCIPLINARY RESEARCH LABORATORIES

Interdisciplinary research laboratories and centers in AMO science and engineering-related areas at universities bring researchers and students together from different disciplines. Formation of such successful facilities has gained from models of joint funding including from state governments and industry. This has enhanced economic development through the state governments' connections with industry and workforce development. In such facilities, students benefit from direct exposure to broader perspectives than just their coursework selection, in line with their career development goals in industry as well as interdisciplinary research in academia. Such centers also enhance opportunities for external fundraising for faculty who want to launch new interdisciplinary research initiatives.

Successful examples of this include the Institute of Optics at the University of Rochester and the Rochester Regional Optics, Photonics, and Imaging Accelerator Program. They benefited from $1.88 million federal funding initially, to help speed the growth of 50 small and medium-size companies, with an additional $200,000 in state support and $700,000 in support from private organizations. Moreover, since 2012, the state of New York has invested $6.1 billion in the economic development of key industries in the Finger Lakes region, including photonics. This "Start-up New York" offers new and expanding photonics companies access to university campuses and to advanced research laboratories, development resources, and experts in key industries. The research environment in these facilities introduces students to interdisciplinary research opportunities as well as to job opportunities in industry.

The Optical Science and Technology Center, the University of Iowa Microfabrication Facility, and the Central Microscopy Facility represent current examples of the original $25 million investment by the state of Iowa in 1987 in interdisciplinary university-based research for laser applications in physics, chemistry, and engineering. This original investment further spurred laser applications in life sciences and the development of companies using optics and photonics tools as well as economic development.

There are other examples that follow this common theme of joint federal, state, and industrial funding. The University of Central Florida (UCF) hosts the Center for Research and Education in Optics and Lasers (CREOL), the largest of four research centers within The College of Optics and Photonics, and the foundational element of the College. In 1986, the Florida legislature acted to provide $1.5 million of annually recurring funds to the UCF budget to support CREOL. In 2007, UCF honored Charles Townes, Nobel Laureate and co-inventor of the laser, by establishing the Townes Laser Institute (TLI) with $4.5 million in funding from the state of Florida. Associated with CREOL, TLI is dedicated to the development of the next generation of laser light engines for applications in medicine, advanced manufacturing, and defense. The University of Arizona's College of Optical Sciences (OSC), established in 1964, has been an innovation front-runner for 50 years, with award-winning students, researchers, and industry partners. OSC is funded by the state of Arizona as part of the university, and is supported by contracts from industry and government. The state of Montana—particularly in the city of Bozeman—has encouraged graduates of Montana State University to start optics companies with funding and tax incentives. More than 30 companies are thriving in Bozeman today.

## FINDINGS AND RECOMMENDATIONS

**Finding:** Other scientific fields, such as the life sciences, have tremendously benefited from AMO science and its tools, as highlighted by single-molecule fluorescence microscopy and adaptive optics being used for super-resolution cellular imaging in near-native conditions. Subsequent advances in synthetic chemistry and materials science have dramatically improved the reach and impact of AMO science and its tools going beyond traditional AMO sciences. Yet, the cross-fertilization between AMO and other fields is not yet occurring at the highest speed possible because of lack of outreach in terms of awareness and availability of the new tools, techniques, and technologies.

**Recommendation: Federal agencies should improve the availability and raise the awareness of the latest AMO technologies for researchers in other fields**

**of science. Additionally, agencies should create funding opportunities to bridge the latest AMO technologies to other disciplines, specifically targeting early adopters.**

**Finding:** Economic development results from AMO-related science and engineering. As exemplified by the University of Rochester, the University of Iowa, the University of Central Florida, the University of Arizona, and Montana State University, state-sponsored centers of excellence in AMO-inspired fields bring researchers and students together from different disciplines in universities, allowing state governments to make connections with industry and thereby promote workforce development. Students at universities benefit from direct exposure to a broader perspective for their coursework selections by direct exposure to what is needed for a career in research and development in industry. This also promotes interdisciplinary research at universities and enhances opportunities for external fundraising for faculty launching new interdisciplinary initiatives.

**Recommendation: State governments should encourage the exploitation of opportunities to compete for economic development in AMO-related science and engineering user facilities at universities using state funding and/or industrial joint support.**

**Finding:** The discussions of engineered quantum matter in Chapters 2 and 4 describe an important emerging field that brings together several disciplines of AMO physics to substantially increase the interaction between material and electromagnetic quantum states. There is great potential for a collaboration between scientists and industry on translational technologies that could miniaturize and scale up a wide range of laboratory-based quantum sensors, including optical clocks and frequency combs. This advance will require a significant increase in the availability of modern advanced photolithography for nanophotonic structures in Si and III-V materials. In addition, students in AMO would benefit greatly from centers dedicated to doctoral training in quantum technologies, modeled on the Centres for Doctoral Training funded by the Engineering and Physical Sciences Research Council in the United Kingdom.

**Recommendation: The National Science Foundation and Defense Advanced Research Projects Agency should create funding opportunities that target strong multidisciplinary collaboration between academia and industry to transfer current e-beam lithography methods in engineered quantum matter to advanced photolithography pilot lines.**

**Recommendation: The National Science Foundation Research Trainee Program should be expanded to ensure that the next generation of post-doctoral fellows are prepared to handle research and innovation challenges across the engineering and physical sciences landscape, particularly in quantum engineering.**

**Recommendation: The federal government should provide funding opportunities for basic research that enables the development of industrial platforms, such as foundry offerings, to support the integration of photonics and engineered quantum matter.**

**Finding:** Astronomical observations have exposed significant shortcomings in our understanding of AMO science that will require significant scientific advances to address. In order to maximize the benefits of ground-based and satellite-based observations, new contributions from AMO theory and experiment are needed to classify the species observed and to understand in detail the elementary atomic and molecular processes occurring in astrophysical environments.

**Recommendation: The National Science Foundation, Department of Energy, and National Aeronautics and Space Administration should support a strengthened community of faculty with the capability to carry out laboratory-based experiments, to develop theory, and to carry out computations in order to maximize the payoff from astrophysical observations and to encourage enhanced support from other funding agencies.**

# 8

# Atomic, Molecular, and Optical Science: Part of the U.S. Economic and Societal Ecosystem

In the preceding chapters, the committee has highlighted the amazing achievements of atomic, molecular, and optical (AMO) science over the past decade, and shown the opportunities these present for future scientific discoveries and new technologies. Recognizing, however, that AMO science does not get done in isolation from the economic and societal structures in which the community operates, in this chapter, the committee examines the state of the field of AMO science in relation to these structures. In similar vein, AMO science is carried out in the global arena, with broad and interdisciplinary reach. We discuss funding, education, workforce development, broad demographic participation, and the global positioning of U.S. AMO science. We use trends over the past decade to take stock of how AMO science is doing with regard to these criteria, and present strategies for confronting challenges and taking advantage of the opportunities identified.

Several factors have contributed to the eminence the United States has enjoyed in AMO science over many decades. These include sustained government funding, extensive investments by academic institutions and industrial research centers, effective translation of AMO research to commercialization and products, and a vibrant, engaged community of scientists worldwide. But AMO science in the United States can also better avail of opportunities to grow its numbers by engaging a broader representation of the changing U.S. population, to maintain and expand funding sources and to ensure that international participation in the U.S. scientific enterprise remains open to citizens of all countries. These topics are explored in this chapter.

## INVESTMENTS IN AMO RESEARCH: FUNDING, COLLABORATION, AND COORDINATION

### Federal Funding

Spending on AMO-related research is an important measure of the opportunities in the field, and of U.S. competitiveness and leadership. In addition to support from academic institutions, industrial partnerships, and private foundations, AMO sciences enjoy substantial federal funding. In constructing the profile for how AMO science is funded in the United States, the committee reached out to the following agencies that have AMO science within their portfolio: the National Science Foundation (NSF), the Department of Energy (DOE), the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and a number of arms of the Department of Defense (DoD)—the Defense Advanced Research Projects Agency (DARPA), the Air Force Office of Scientific Research (AFOSR), the Office of Naval Research (ONR), and the Army Research Office (ARO).

In order to understand the impact of federal funding on AMO research, the committee set out to answer the following questions pertaining to aggregate AMO spending across all programs, with the goal of determining if funding for AMO sciences has remained robust over the past decade:

- What was the absolute number of dollars spent on AMO research each year over the past decade at the queried agency?
- What was the distribution of grant size each year for the past 10 years?

Since the committee also attempted to understand opportunities for early career scientists to secure federal funding for their research, the agencies were also asked:

- Over the past decade, how many awards go to grantees each year as a function of the grantee’s time past Ph.D.?

The committee asked for this to be divided into three time bins: 5 years after Ph.D., 10 years after Ph.D., and beyond 10 years after Ph.D.

The committee received detailed responses from several, but not all, agencies, and in some cases, with caveats. These are shown in Table 8.1. The trends for funding in the aggregate, based on the data in Table 8.1, are shown in Figure 8.1. The total amount of dollars (in millions) spent on AMO-related research is plotted for each of the past 10 years, from 2008 to 2018. Each data point is the sum of spending reported by all the agencies that provided the data. This plot is based on the “sum” row of Table 8.1, where annual spending is broken down by agency.

**TABLE 8.1** Funding Histories in AMO Science (2008-2018) (millions of dollars)

| | DoD | | | | | | | DoD/DOE/NIST/NSF | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Year | AFOSR[a] | ARO | DARPA[b] | ONR | DOE[c] | NIST[d] | NSF[e] | As-Spent Total | Deflator[f] | FY2018 $ |
| 2008 | 4.00 | 8.55 | 9.6 | 1.55 | 14.70 | 76.86 | 22.15 | 137.41 | 0.854 | 160.86 |
| 2009 | 4.00 | 11.29 | 17.68 | 3.9 | 20.10 | 79.78 | 22.25 | 159.01 | 0.861 | 184.75 |
| 2010 | 4.00 | 7.03 | 11.44 | 2.2 | 20.10 | 79.46 | 23.55 | 147.78 | 0.871 | 169.73 |
| 2011 | 4.00 | 9.29 | 57.58 | 2.12 | 21.60 | 80.74 | 23.07 | 198.39 | 0.889 | 223.2 |
| 2012 | 10.00 | 8.51 | 29.2 | 2.19 | 20.10 | 83.32 | 23.02 | 176.33 | 0.906 | 194.64 |
| 2013 | 10.00 | 9.74 | 33.92 | 2.73 | 20.10 | 85.07 | 21.01 | 182.56 | 0.922 | 198.05 |
| 2014 | 10.00 | 13.04 | 11.65 | 3.96 | 21.00 | 86.34 | 21.08 | 167.08 | 0.939 | 177.89 |
| 2015 | 10.00 | 12.05 | 8.32 | 3.08 | 20.40 | 87.73 | 22.19 | 163.76 | 0.949 | 172.51 |
| 2016 | 10.00 | 9.62 | 23.4 | 2.75 | 21.60 | 87.81 | 22.17 | 177.35 | 0.960 | 184.8 |
| 2017 | 10.00 | 10.11 | 2.85 | 2.92 | 21.90 | 88.96 | 22.63 | 159.37 | 0.978 | 162.97 |
| 2018 | 10.00 | 11.05 | 7.27 | 3.45 | 23.40 | 90.82 | 22.54 | 168.54 | 1.000 | 168.54 |

[a] AFOSR mentioned the cost of only two major programs: the Atomic and Molecular Physics program at about $4 million per year, and the Ultrashort Pulse Laser-Matter Interactions program, which started in 2012, at about $6 million per year. Funding for MURI programs, some of which is directed to AMO research, is not included by AFOSR nor ONR, although it is included by ARO.

[b] DARPA data for 2008 is a lower bound that was inferred from the Services, and not provided by DARPA. Note that DARPA programs do not represent generic (or core) funding for AMO, but are focused initiatives that come and go.

[c] DOE did not provide actual numbers; instead, these figures represent rough estimates from a bar graph that they did provide, reduced by a factor of 97 percent, as they instructed.

[d] NIST data extrapolated from AMO2010: $70 million in 2005 adjusted using year over year CPI inflation rates, as published by the Federal Reserve Bank of Minneapolis (see https://www.minneapolisfed.org/community/financial-and-economic-education/cpi-calculator-information/consumer-price-index-and-inflation-rates-1913).

[e] Does not include Plasma or QIS programs.

[f] As calculated from rates published by the Federal Reserve Bank of St. Louis, https://fred.stlouisfed.org/release/tables?rid=53&eid=41158.

Figure 8.1 and Table 8.1 show that federal funding for AMO-related science over the past decade has more or less held steady, but with significant year-to-year fluctuations. The largest year-to-year variations in AMO spending occurred at DoD (primarily in DARPA and to a lesser extent at the Services). DARPA has a large budget with significant changes in how funds are directed from time to time. Prior to 2003, for example, relatively little AMO-related basic research was funded by DARPA. Periodic increases in AMO funding can be ascribed to program officers who identify specific opportunities or target particular areas, and direct funding accordingly. Furthermore, Figures 8.1b and 8.1c show that spending (and hence budgets) for AMO research by NSF and DOE have remained close to flat over the past decade, in 2018 constant-dollars, while NIST has increased almost steadily, and as mentioned DoD has had large year-to-year fluctuations.

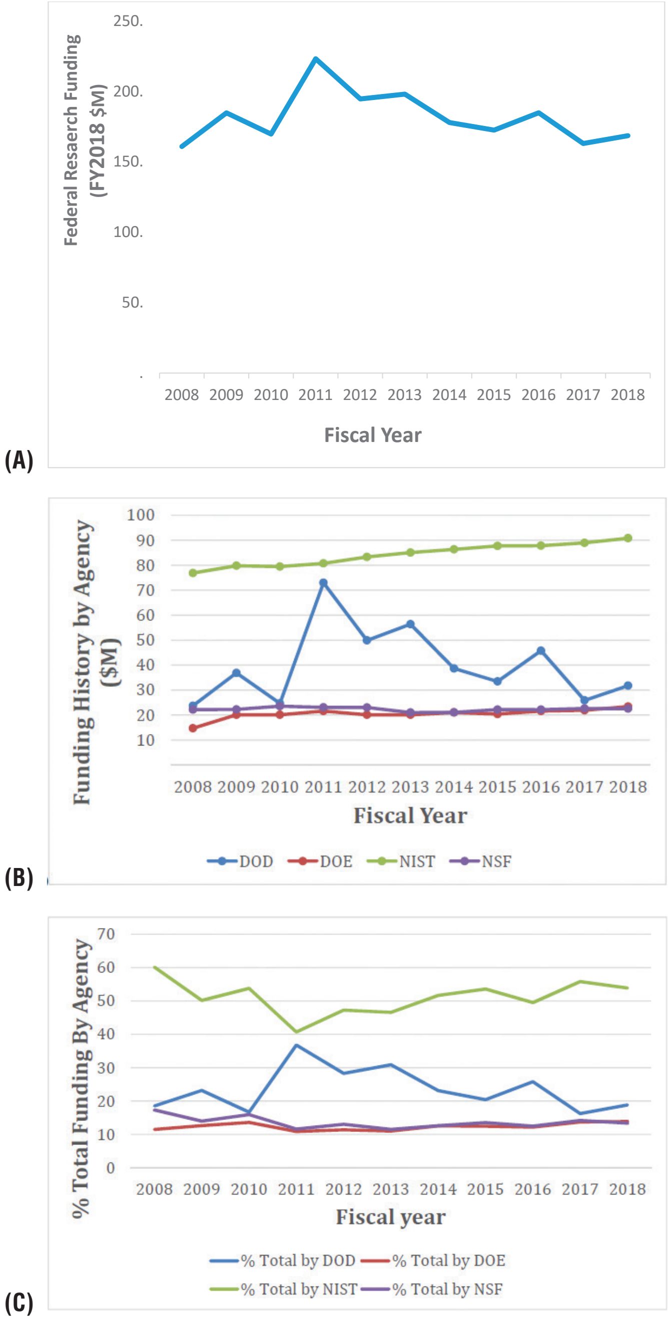

**FIGURE 8.1** Annual trends for funding of AMO-related research by (A) the sum over agencies listed in Table 8.1, (B) the agencies broken out as indicated, and (C) the agencies shown as a percentage of total spending.

Traditionally, AMO physics has been carried out by small groups in table-top-scale experiments. While this is still at the core of AMO experiments, there are increasingly opportunities for AMO science to contribute to other areas of science in larger, multidisciplinary teams that require funding modalities that need to adapt to these needs. Examples of these are the Laser Interferometer Gravitational-Wave Observatory (LIGO) project, and on a smaller scale, experiments like ACME and Axion Resonant Interaction Detection Experiment (ARIADNE). These are elegant experiments that use the techniques of AMO to probe astrophysics and fundamental properties of known and yet undiscovered particles.

Efforts such as these highlight the need for interagency funding modalities with longer horizons. Strong interagency coordination to achieve optimal balance for funding between single investigators and collaborations with varying sizes would be very beneficial for availing of these opportunities and for facilitating the discovery potential of AMO. Flexibility in funding structures will be imperative, responding to both existing and rising opportunities in a timely fashion. Many of these bigger-than-table-top-scale experiments are in the domain of questions of fundamental interactions traditionally explored through DOE support. Another area DOE has become increasingly interested in is helping shape the future of quantum information science and technology. It will be important for DOE to work together with NSF, NIST, DoD, and even NASA to identify fundamental physics questions and applications that can be best addressed, both within the DOE National Laboratories and outside, with investment in quantum and AMO science. As another example, to build powerful quantum machines and use them to solve important scientific and technological problems will require teams working between large facilities to address material and technical challenges and smaller sized groups to tackle fundamental issues in quantum information science.

Another concern is the high threshold to entry for early career AMO scientists. As AMO laboratory programs grow more expensive to seed, it gets prohibitively expensive for smaller colleges and universities to hire AMO scientists as assistant professors. A likely contributor is the ballooning startup costs resulting from the cumulative costs of the many custom pieces of equipment that are required to put together increasingly complex and precise experiments. A possible solution may be a new funding model for such home-built pieces of equipment that do not fit into typical NSF Major Research Instrumentation Programs. Recognizing startup costs as a serious barrier that has a negative impact on the breadth and diversity of students with training in AMO laboratories, something that has been identified as a national need (see the section below, “Workforce, Educational, and Societal Needs”), the committee tried to determine how funding is distributed among early, mid-, and late-career researchers, but could not consistently access such data. The committee learned, for example, that CAREER awards—for outstanding scientists at the beginning of their academic careers—made up 6 percent of all awards funded by the NSF AMO program, averaged over the past decade. According to current membership data collected by the American Physical Society (APS; see the section "Workforce, Educational, and Societal Needs"), 47 percent of scientists who identify with the Division of Atomic, Molecular, and Optical Physics (DAMOP) are students. While NSF CAREER grants are only awarded to the very best of new incoming faculty, and not all of those DAMOP students will even go into academic careers, the small fraction of these grants relative to the numbers of young people in the field may point to the need for directing more funding to early career investigators. Because we recognize that this is not a strong, data-driven correlation between a small subset of early career funding and early career membership to the DAMOP, this points to the need for a separate study to determine the optimal level of funding for starting faculty.

A possible modality for supporting early career AMO academicians could be prestigious postdoctoral fellowships that can be ported between institutions. Such fellowships could be awarded to postdoctoral scholars before they start faculty positions, and could be used to defray startup costs that many smaller institutions cannot incur.

### Interagency and Industrial Connections of AMO Science

AMO research is a worldwide activity, with significant investments in AMO science in Europe, Asia, and Australasia. AMO science is also a multidisciplinary enterprise; strong connections to other areas and to industry are highlighted in Chapters 6 and 7. Consequently, it is important to support and amplify this interconnectivity both through international collaborations and in the context of multiple U.S. federal funding agencies, state-level funding opportunities, industry, and education and outreach to engage the public that supports scientific research.

Within the United States, AMO research is largely funded by several federal agencies and is a significant component of many industries. AMO-trained scientists populate virtually every type of commercial undertaking, from manufacturing to financial services. This has grown to the point that there is now significant "back-action": it is important for the AMO community to learn from industry on their pressing needs for workforce and how best to train students to meet these needs. Close working partnerships between AMO and industry will be critical for technology transfer and development of innovative products. It can also strengthen support for fundamental science. Strengthening partnerships among the different federal funding agencies and between agencies and industry will further cement these connections and increase the immediate societal impact of AMO-based training and technologies.

Within agencies, there is support for interdisciplinary research activities. The NSF AMO program, for example, co-funds research with nearly a dozen other programs across NSF. Within and across DoD agencies there is also significant interdisciplinary and cross-program funding. However, across multiple different agencies there is a larger challenge. There are specific instances of programs where NSF, DoD, and DOE have (pairwise) co-funded programs, but this is more the exception than the rule. As highlighted in preceding chapters, there will be great benefit to all parties to make this easier or more natural to do when the situation arises.

## Translation of AMO Research to Industry

In Chapter 7, we discussed the impact that AMO has had on society through both widely publicized discoveries and technology transfer to industry—through start-ups, research and development (R&D) collaborations, and intellectual property licensing through universities. A particularly vivid example is provided by the telecommunications industry, which had to dramatically reduce losses in optical fibers, improve the power and frequency stability of lasers and the sensitivity of photodetectors, and then field these technologies across the globe on cost-effective and reliable platforms. Higher levels of integration have generally enabled scaling to much higher volumes at still lower costs (i.e., “Moore’s law”), and integrated photonics based on III-V semiconductors rapidly grew into a USD $0.5 billion to $1.0 billion industry driven by demand for Internet connectivity. In parallel, the field of silicon photonics was launched in the 1980s and 1990s by academic researchers who were interested in harnessing submicron silicon-on-insulator optical structures to create first passive (waveguides, splitters, optical fiber couplers) and then active devices (modulators and detectors) for applications ranging from data transceivers to labs-on-a-chip. The data communications industry—responsible for fielding interconnect networks for data centers and high-performance computers—followed this research closely, and by the turn of the century startups began to appear with the intention of commercializing this research.

This new era of high-commercial-volume, high-reliability, low-cost datacom photonic circuits—now a USD $1 billion industry that is likely to grow much faster than telecom—brings a tension between the different approaches used by academia and industry.

- As photonics has evolved to ever larger scales of implementation and adoption, reliability of the underlying components has continued to increase in importance. In academic papers and conferences, the very best results are emphasized. But in industry, public dissemination of product capabilities generally makes a more conservative pitch. Industry has learned how to build in reliability at the substrate level, and this information is widely available to the academic community.

- The software and hardware tool chains that are used by industry to design large-scale photonic circuits are adapted from those used by the CMOS industry and are quite powerful and sophisticated. Graduate schools in electrical engineering have been teaching their students to use these tools for more than 20 years, but very few AMO physics departments have begun to follow suit.
- Similarly, converting a scientific experiment into a technology involves a deep awareness of design, integration, packaging, and reliability. These skills have traditionally not been taught in AMO research laboratories, so industry must engage in a significant amount of on-the-job training to bring their new, young scientists up to speed. There are now a few academic centers of excellence with this sort of training in mind. For example, the Engineering and Physical Sciences Research Council is funding the University of Bristol's Centre for Doctoral Training in Quantum Engineering, which is designed to educate graduate students in modern manufacturing and fabrication techniques to speed product development in this new field. In the United States, NSF has launched the Research Traineeship Program with the intention of performing a similar function.

Bridging this gap between current practices and the goal of educating students in the methods and tools of importance to industry is well within the capabilities of the nation's universities.

## AMO Science Internationally

There is good evidence that the U.S. investments in R&D are declining relative to other parts of the world (see, e.g., Figure 8.2), even as the United States contributes 19 percent to the overall increase in worldwide expenditures on R&D (NSB Science and Engineering Indicators 2018). While these were not AMO-specific, we can expect that AMO science follows similar trends. Attempts at collecting country-specific data on international funding of AMO sciences proved to be futile. But anecdotally, we see that worldwide investments in AMO science are growing at a faster pace than in the United States. The committee examined AMO opportunities in other parts of the world in order to identify possible strategies that could be used in the United States. Of particular note were the extensive investments in AMO sciences and technologies in Europe through Framework Programmes for Research and Technological Development and the Quantum Flagship, a large-scale research and innovation initiative. In addition to national programs in European Union (EU) member nations, Europe also has network funding mechanisms

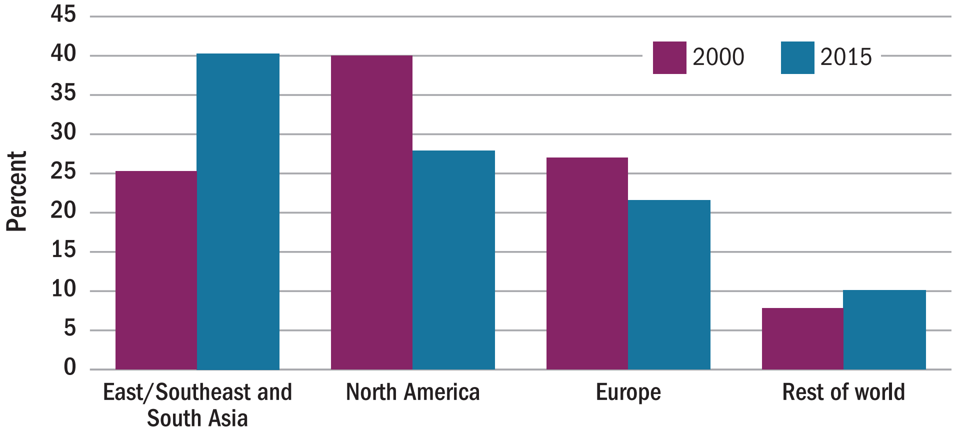

**FIGURE 8.2** Worldwide R&D expenditures by region. NOTE: East/Southest and South Asia includes China, Taiwan, Japan, South Korea, Singapore, Malaysia, Thailand, Indonesia, Phillippines, Vietnam, India, Pakistan, Nepal, and Sri Lanka. SOURCE: Science and Engineering Indicators 2018, Cross-National Comparisons of R&D Performance, Chapter 4.

through which multiple funding organizations from multiple countries coordinate research in quantum information sciences. These methods of support could serve as models for the United States as the need for greater interagency funding grows. One avenue we see for remaining competitive and using the available resources most effectively would require collaborations between U.S. agencies not just among one another but also internationally.

The committee used publication in peer-reviewed journals as one measure of the volume of AMO research performed in various countries. We are aware that the quality of publications can vary, but total number of publications should be a reasonable measure of engagement in AMO research. In absolute number of publications, China and the United States led all other countries, as shown in Figure 8.3a. However, when the total number of publications are scaled by population for each country, the authorship per capita placed Germany in the lead, as shown in Figure 8.3b. A similar analysis of authorship per gross domestic product (GDP) is shown in Figure 8.3c.

Using these publication trends over the past decade as a proxy for research volume, we see that there has been sharp growth in the number of publications originating from researchers at Chinese institutions compared to all other leading countries. With the exception of China and to a lesser extent the Russian Federation, research publications per capita or per GDP show a declining trend over the past decade. It is also worth noting that several members of the EU—Germany, France, Italy, and the United Kingdom—are among the top 10 countries with

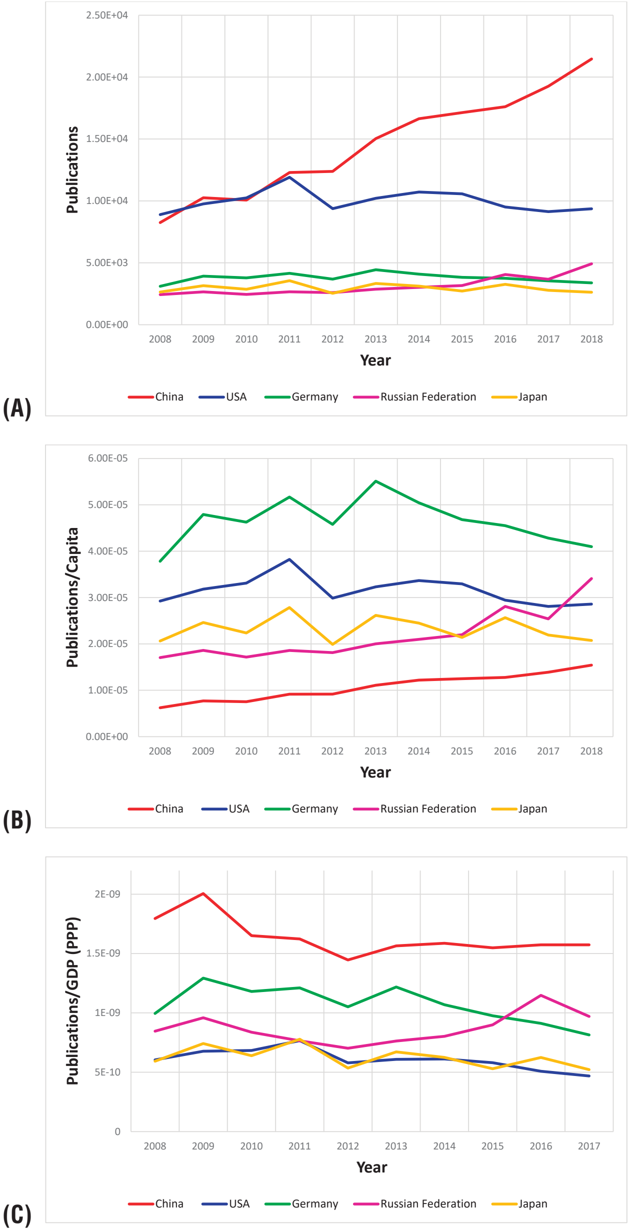

**FIGURE 8.3** Publication trends by country for the top five countries producing the largest number of publications in atomic, molecular, and optical-related research in peer-reviewed journals (A); for these same five countries, ordered by the largest number of publications per capita (B); and again for these same five countries ordered by the largest number of publications per GDP (C), where GDP is corrected for purchasing power (PPP – purchasing power parity). The large variations for the Russian Federation are related to the Russian financial crash (2014 to 2017).

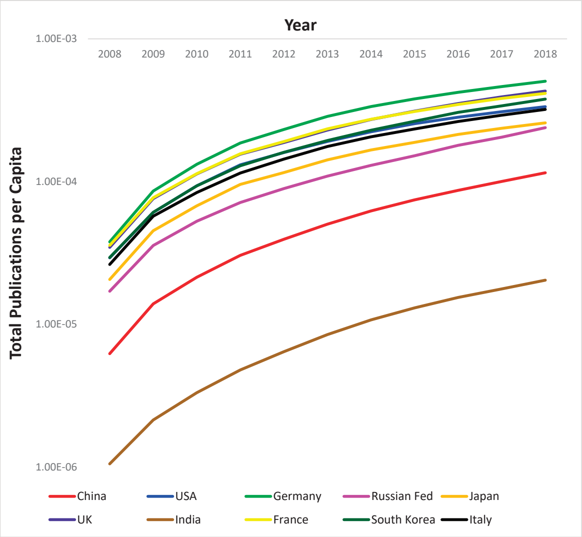

**FIGURE 8.4** Top 10 countries ranked by per capita publications of atomic, molecular, and optical-related research in peer-reviewed journals, shown on a logarithmic scale to highlight the large variations.

the largest number of publications per capita in AMO-related sciences, as shown in Figure 8.4.

## WORKFORCE, EDUCATIONAL, AND SOCIETAL NEEDS

### Education and Workforce Development

Looking to the future, the health and vibrancy of the AMO ecosystem depends on—and contributes to—the development of a technical workforce prepared for 21st century challenges. A significant measure of the workforce of the future is given by current trends in education and employment. To determine the educational trends in AMO science, the committee studied data from the American Institute for Physics (AIP).

Figure 8.5 shows the number of Ph.D. degrees conferred in physics by field of study for the years 2013 and 2014 combined. Of the 1,773 Ph.D.s granted at U.S. institutions of higher education, 99 Ph.D.s were in atomic and molecular physics (5.6 percent) and 79 Ph.D.s were in optics and photonics (4.5 percent). Atomic and molecular physics plus those in optics and photonics (AMOP) combined with 178 is tied at third place for the largest subfield of physics. While the number of physics Ph.D.s rose 68 percent from 2002 to 2015, AMOP Ph.D.s rose by only 52 percent. Figure 8.6 shows the number of Ph.D.s granted in physics at U.S. institutions, and also the sum of Ph.D.s in AMOP for the years 2002 through 2015.

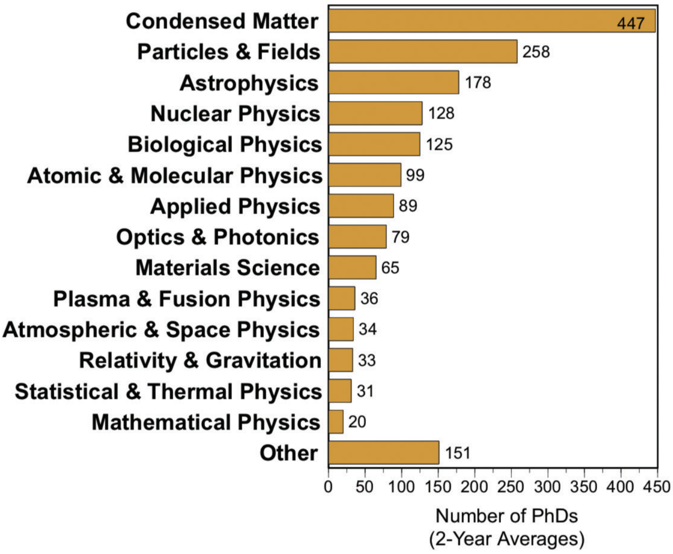

**FIGURE 8.5** Number of Ph.D.s granted at U.S. institutions for the years 2013 and 2014 combined. SOURCE: Courtesy of the American Institute of Physics.

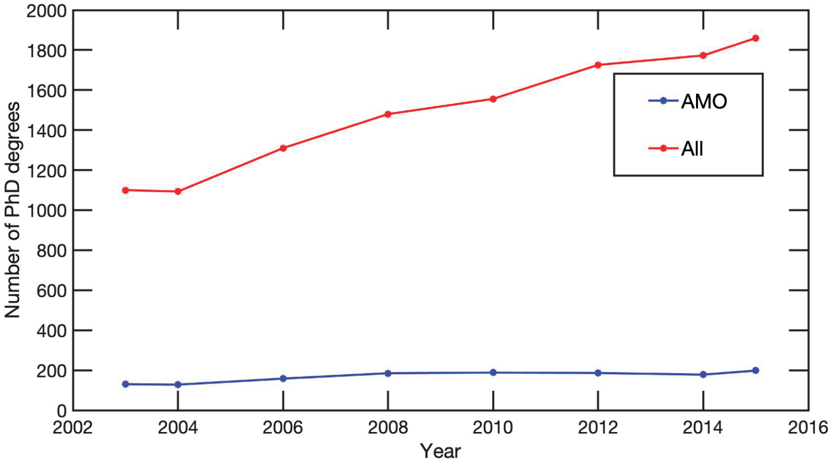

**FIGURE 8.6** Number of physics Ph.D.s granted at U.S. institutions. The red curve shows degrees awarded; the blue data shows degrees in atomic and molecular physics, plus those in optics and photonics. Since 2015, the American Institute of Physics has changed the way these categories are defined, so we are not able to monitor the trends with more recent data. SOURCE: Courtesy of the American Institute of Physics.

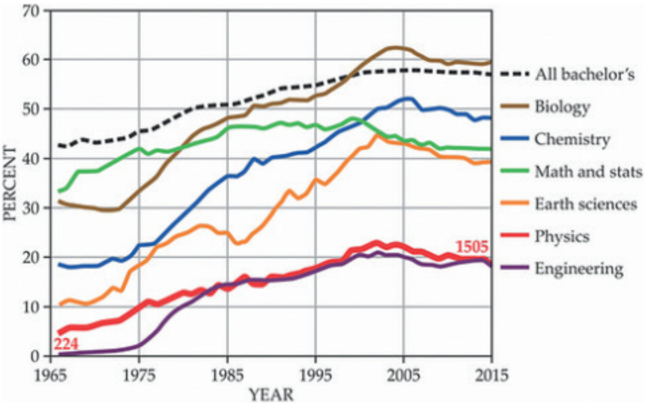

**FIGURE 8.7** Science, technology, engineering, and mathematics bachelor's degrees earned by women in the United States, 1965-2015. SOURCE: Courtesy of the Integrated Postsecondary Education Data System and the American Physical Society.

To evaluate whether there were missed opportunities to broaden participation in the workforce, the committee studied as an example education trends for women and underrepresented minority (URM) students. We delve into this topic a bit more in the following section on demographics. Figure 8.7 shows the trends for the percentage of women earning science, technology, engineering, and mathematics (STEM) degrees in the United States. The committee notes that women now earn nearly 60 percent of all bachelor's degrees in the United States (see NCES 2019-038), but comprise just about 20 percent of physics majors in bachelor's programs, a number that has remained static over the past decade (see AIP Report on Women in Physics and Astronomy, 2019).

Similar data were not available for URMs, but experience at our home institutions strongly suggests that the participation of those groups is even smaller. Bridge programs have increasingly shown promise to enhance URM participation in physics, from the longstanding examples like Fisk-Vanderbilt to the more recent APS Bridge programs. Particularly promising are when programs start earlier, while students are still in their undergraduate years, with Cal-Bridge showing very positive outcomes. We encourage others to follow these models, or collaborate with them.

Taken together, this presents a very significant opportunity—an imperative even—to increase the number of women and URM students training to be physicists. In order to achieve greater representation, a number of systemic barriers faced by women and URM students must be overcome. Some of the challenges women face as physicists, ranging from implicit bias to male-dominated subcultures, are discussed in an excellent article by Blue, Traxler, and Cid that appeared in the March 2018 issue of *Physics Today*, (https://doi.org/10.1063/PT.3.3870).

A large component of AMO scientists in the United States comprises those not born in the United States. There is a longstanding tradition of talented AMO scientists coming to the United States from other countries—as students or thereafter—and building productive careers here. Some of the most outstanding American citizens practicing AMO science were born outside the United States. NSF's "Science and Engineering Indicators" report shows that foreign-born scientists make up about half of the Ph.D. holders in "physical sciences," but anecdotally it seems that intellectual immigrants contribute disproportionately to AMO science, even relative to this figure.

The need to attract and retain brilliant foreign-born scientists is critical to the continued health of AMO science, and the American scientific enterprise more generally. It is, therefore, imperative to preserve—and indeed improve—mechanisms by which non-U.S.-born scientists can contribute to U.S. scientific enterprise, and to ensure that the United States remains as welcoming a place to pursue AMO research as ever.

As part of our data-gathering efforts for this report, the committee also conducted two town hall meetings, held during the annual meetings of the APS and the Optical Society of America (OSA), respectively. The APS has more than 55,000 members, including physicists in academia, national laboratories, and industry in the United States and throughout the world. The Division of Atomic, Molecular, and Optical Physics (DAMOP) is a unit of the APS; its membership is represented in Figure 8.8. As noted below, other APS divisions are increasingly connected to DAMOP ideas, and conversely.

At a town hall meeting held at the 2018 DAMOP annual meeting, prominent members of the AMO community raised concerns, but also expressed enthusiasm for the achievements of AMO science over the past decade, and optimism for the future. Chief among the concerns raised were the funding trends that had not kept up with the growing AMO activities, shown in Figure 8.1, and the consequent danger of U.S. scientists losing their competitive edge. The very small number of theoretical AMO physicists in the United States was raised as a concern. Another was that as many AMO research group sizes have grown, and been supported by more project-driven funding sources, these might be supplanting curiosity-driven research, which is the mainstay of discovery. It was also noted that the short (3 years or fewer) funding cycle for most federal grants makes it very difficult to maintain and augment infrastructure in research groups. Despite these concerns, there was also wide recognition and celebration of the role AMO science has played—and is anticipated to continue to play—in some of the most important scientific and technical advances of the past decade. These include developing platforms and tools for quantum computing and quantum information science more broadly; novel

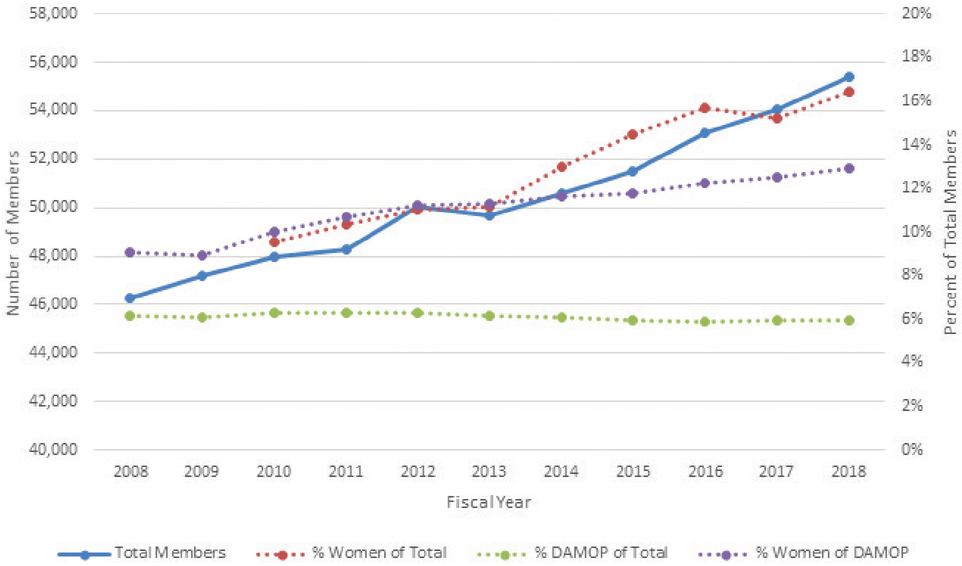

**FIGURE 8.8** Demographics of the membership of the American Physical Society (APS). Membership in the Division of Atomic, Molecular, and Optical Physics (DAMOP) relative to membership in the APS as a whole, and fractions of women members. The blue curve shows the total membership of the APS, corresponding to the left y-axis. The remaining curves show percentages, corresponding to the right y-axis, for the fraction women members relative to the total membership (red), the fraction of DAMOP scientists relative to all members (green), and the fraction of DAMOP members who are women (purple). SOURCE: APS data.

biomedical diagnostics; advancing the precision frontier with the development of clocks, further improvements in metrology, and the detection of gravitational waves; synthesizing new forms of matter; and observing light-matter interactions at unprecedented high intensities and speeds.

An important piece of feedback that the committee collected from industry on workforce training is the rising need for AMO-trained students, especially in the rapidly evolving fields of integrated photonics and quantum information science and technology. This growing need for technically trained workers who have had AMO-related experience in laboratories during their education is easily understood: industry needs most closely match AMO training. Thus, trained undergraduate and master's degree students with sufficient knowledge in AMO are actively sought by industry, particularly those who have had a reasonable exposure to AMO laboratories. The laboratory experience is invaluable since no classroom or textbook can prepare a student for the laboratory, where the full complexity of apparatus manifests and interacts with the environment in uncontrolled ways. This national need illustrates the opportunity for the AMO community to improve upon the current education curricula and provide innovative laboratory training for students.

The need for more resources to train AMO students extends beyond the need for bachelor's (or higher) degree holders. An underestimated, but important, sector of a technical workforce is the skilled technician. Skilled technicians with "golden hands" in the laboratory—essential resources for scientists in industry, academia, national laboratories, and government—can often be extremely productive with less than a full formal education. The skill sets of qualified technicians readily translate from academia to industry, and just as easily from industry to academia.

Many talented technicians have completed a few relevant community college courses, polytechnic training, or in some cases training for military technical certification. Not only do such programs provide an important source of critical help for working scientists, they also provide a low-barrier entry path for potential new scientists, allowing individuals who may otherwise not join the technical workforce to gradually build a career in science through hands-on training rather than a classical 4-year college program. Designing and financially supporting some less traditionally academic paths can be a tremendous resource for technical workforce development. The German apprenticeship model is an example of training highly skilled technicians without requiring a 4-year college degree. A 2017 study published by the American Academy of Arts and Sciences (J. Brown and M. Kurzweil, The Complex Universe of Alternative Postsecondary Credentials and Pathways) examines an array of alternatives to 4-year degree programs.

As noted above, industry has also given clear indication that there is much excitement about AMO sciences and the tools they bring to the U.S. high-tech sector, yet it has proven hard to find workers with the right skillset—of training in both analytic and experimental methods of AMO sciences. Partly this is because AMO-trained physicists are rapidly hired as soon as they are produced. To address this growing opportunity space, coupled with the growing need for more people with this expertise, it is important to find ways to increase the potential workforce. As a step in that direction, the committee studied who are the current practitioners of AMO sciences. This will help us to identify where to look for opportunities to engage others. Parts of the U.S. population that are disproportionately underrepresented in AMO sciences would be one such place.

### Practitioners of AMO Science: People and Demographics

The committee recognizes the importance of creating a diverse workforce through inclusive practices in order to harness the full potential of all possible scientists who could contribute to the AMO endeavor. To this end, the committee tried to determine the level of participation of women and URMs in AMO science, and what barriers—implicit or otherwise—may prevent greater participation. The major source for this was the membership statistics of the largest international organization for physicists, the APS.

The APS provided the committee with membership data for the past decade, which is summarized in Table 8.2.

Figure 8.8 shows the membership of the APS for each year between 2008 and 2018 that identified with DAMOP. Specifically, the committee notes that of roughly 55,000 members of the APS in 2018, 3,300 are members of DAMOP, or about 6 percent. The membership of DAMOP has grown roughly at the same rate as the total APS membership. DAMOP does not cover all AMO-related scientists, at least some of whom may identify with other divisions or topical groups, such as the Division of Chemical Physics, the Division of Laser Science, the Division of Physics of Beams, the new Quantum Information Division, or the Precision Measurement and Fundamental Constants Group, or the Few-body Systems Group. In similar vein, there are many other members of the AMO community who do not belong to DAMOP, so the DAMOP numbers underrepresent the full extent of AMO scientists, possibly by as much as a factor of two. But since we were able to acquire data for DAMOP, some statistical trends can be extracted from that data.

In particular, the committee finds that in 2018, for example, women constituted about 13 percent of the DAMOP membership, while about 47 percent of the total are student members. The students represent a potential future workforce, while

**TABLE 8.2** Demographics of American Physical Society Membership

| Year | Total Members | Women Members[a] | DAMOP Members | Women DAMOP *Members*[b] |
|---|---|---|---|---|
| 2008 | 46,269 | not available | 2,837 | 257 |
| 2009 | 47,189 | not available | 2,885 | 257 |
| 2010 | 47,947 | 4,573 | 3,023 | 302 |
| 2011 | 48,263 | 4,996 | 3,052 | 327 |
| 2012 | 50,055 | 5,521 | 3,156 | 354 |
| 2013 | 49,653 | 5,524 | 3,072 | 347 |
| 2014 | 50,578 | 6,562 | 3,096 | 361 |
| 2015 | 51,523 | 7,466 | 3,051 | 359 |
| 2016 | 53,096 | 8,313 | 3,114 | 382 |
| 2017 | 54,029 | 8,207 | 3,235 | 404 |
| 2018 | 55,368 | 9,093 | 3,303 | 427 |
| 2019 | 55,160 | 9,704 | 3,185 | 420 |

[a] Roughly 10 percent of APS members do not self-report gender information, each year.
[b] Roughly 5 percent of APS AMO members do not self-report gender information, each year.

the percentage of women speaks to an underrepresented community whose greater participation could help avert the shortfalls expected relative to workforce needs.

A striking statistic that became evident in the APS data is that historically women are disproportionately underrepresented among elected fellows of the APS. Although, as mentioned, in 2018 women comprised 13 percent of the DAMOP membership, only 1.4 percent of APS-DAMOP members are female fellows. Men, on the other hand, comprised 81 percent of DAMOP membership, with 17.5 percent APS-DAMOP members being male fellows. In other words, 11 percent of women members are elected fellows of the society, compared to 22 percent of men members, meaning that men have been twice as likely to be elected fellows as women. While election to APS fellowships is typically reserved for mid- to late-career researchers, and thus may be a lagging indicator of trends, the situation is not improving in recent times, despite active efforts from the community to nominate women researchers. This is one indicator of the numerous barriers women face in being fully equal participants in AMO science (although this pattern is largely similar across subfields of physics). Some of the issues faced by women in STEM fields have been highlighted in the 2018 Consensus Study Report of the National Academies of Sciences, Engineering, and Medicine titled *Sexual Harassment of Women: Climate, Culture, and Consequences in Academic Science, Engineering, and Medicine*.[1] That report examines sexual harassment of women in academic sciences, engineering, and medicine, and concludes that the cumulative effect of sexual harassment damages research integrity and leads to a costly loss of talent in STEM academic fields. The report provides recommendations to academic institutions and the federal government for addressing the pandemic problem of sexual harassment that seriously impacts the participation of women in all STEM academic fields.

Understanding the level of participation by historically underrepresented groups along ethnic and racial lines is particularly challenging since the numbers are small and because data are scant, so statistical methods must be used with caution. In the absence of AMO-specific data, the committee uses national trends in STEM education as a proxy for AMO sciences. Doctoral degrees granted in STEM fields to U.S. students is shown in Figure 8.9.

The NAS Graduate STEM Education report indicates that in 2015, five physics Ph.D.s were granted to Native American and Alaskan Native students, 18 to Black or African American students, and 44 to Hispanic and Latino students, adding up to 67 out of a total of 1,840 doctoral degrees in physics that year. This corresponds to 67/1,840 = 3.6 percent of all physics Ph.D.s awarded to ethnic and racial minorities in 2015. This is consistent with (although not identical to) data collected by the AIP, shown in Figure 8.10.

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[1] https://doi.org/10.17226/24994.

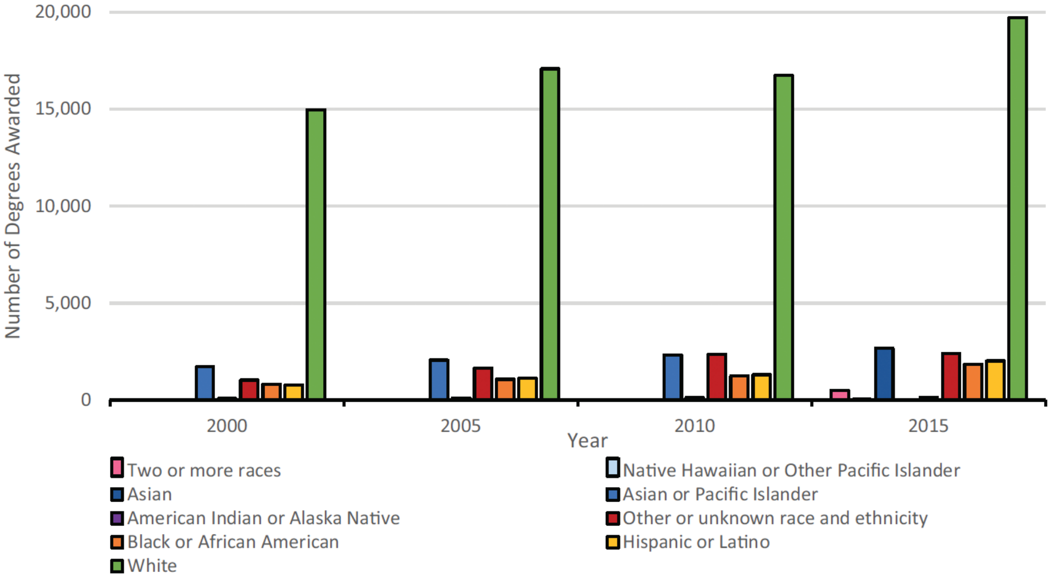

**FIGURE 8.9** Number of doctoral degrees awarded to U.S. students by race and ethnicity over all science, technology, engineering, and medicine (STEM) fields at U.S. institutions. Not shown, but the committee notes separately from that report, that of all STEM doctoral degrees granted, 4.3 percent in 2000 and 4.1 percent in 2015 were Ph.D.s in physics. SOURCE: Reproduced from Figure 2-4 of the NAS Graduate STEM Education report.

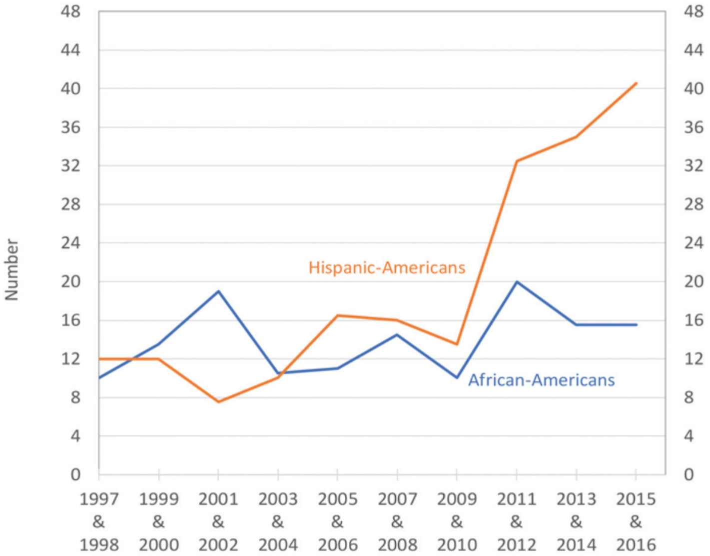

**FIGURE 8.10** Doctoral degrees in physics granted to Hispanic Americans and African Americans, presented as 2-year averages, spanning 1997 to 2016.

One can expect that the demographic trends in AMO sciences are not too different from physics overall. This is of course disheartening, alarming even, given the demographic shifts in the U.S. population where non-whites account for more than 40 percent of the population. On the positive side, this means that there is an enormous talent pool that physics, and correspondingly AMO sciences, could tap in the future.

While there is little doubt that there are opportunities for AMO science to grow its talent pool and increase participation from underrepresented groups, the field currently does overall appear to be slowly growing. From the data shown in Table 8.2, we see that the number of professional physicists who identify as AMO scientists grew over the past decade, but only at about the same rate as APS membership overall. Note that both had year-to-year variations that could be quite large, and almost seem to track one another. These overall increases imply robust interest in AMO sciences, and funding that seems to be keeping pace with growth.

## U.S. Workforce Development and Competitiveness in a Globalizing World

Traditional AMO training focuses on physics; however, the development of quantum technology requires reaching across both academic disciplines and to industry to leverage the impact of AMO. There are existing successful portable funding models in the United States and Europe, such as the National Institutes of Health (NIH)-K99 and European Research Council (ERC) grants, that could be used as models to assist faculty appointment and early career development. For the U.S. to remain competitive in the world, more such portable grant mechanisms would prove valuable. In designing such portable funding models, it will be important to ensure that the level of research effort is compatible with teaching expectations that are standard in the U.S. physical sciences academic community. Other AMO funding agencies should develop similar models that support the transition of AMO theorists and experimentalists into faculty positions.

The AMO workforce has historically been underrepresented in theorists. With the recent cross-fertilization of fields that we have been seeing, we now have more theorists working in AMO than in the past. Few of these, however, are theorists specifically trained in AMO, as opposed to, for example, condensed-matter theorists tackling problems at the intersections with AMO. This is very different than the situation in Europe, and may contribute to the reasons that the rest of the world is rapidly overtaking us in AMO.

Despite the encouraging overall growth seen in the AMO workforce, there continues to be great demand for more of such an AMO technically trained workforce. While the data on workforce needs gathered by this committee through community input are anecdotal, this issue of the need for a technically trained workforce more generally has been studied in great detail in recent National Academies studies. One can look to those studies for guidance in assessing the needs in AMO sciences. Fueled by the ominous and prescient report *Rising Above the Gathering Storm*, development of a technically skilled workforce in the United States has been the subject of a number of studies carried out by the National Academies and professional societies. Four reports are of particular relevance to this study:

- National Academies of Sciences, Engineering, and Medicine. 2018. *Graduate STEM Education for the 21st Century.* Washington, DC: The National Academies Press. https://doi.org/10.17226/25038. This report provided guidelines for creating a generation of students with broad technical literacy and deep specialization in their area of study, acquiring core competencies through the U.S. graduate education system.
- National Academies of Sciences, Engineering, and Medicine. 2017. *Building America's Skilled Technical Workforce.* Washington, DC: The National Academies Press. https://doi.org/10.17226/23472.
- National Academies of Sciences, Engineering, and Medicine. 2016. *Developing a National STEM Workforce Strategy: A Workshop Summary.* Washington, DC: The National Academies Press. https://doi.org/10.17226/21900.
- National Academies of Sciences, Engineering, and Medicine. 2016. *Expanding Underrepresented Minority Participation: America's Science and Technology Talent at a Crossroads.* Washington, DC: The National Academies Press. https://doi.org/10.17226/12984. This report argues the importance of a workforce that is representative of the demographics of the population, and therefore, an increasingly diverse workforce in the United States. A number of recommendations are made to increase preparation, access, motivation, support, and affordability, and for education to close achievement gaps between minority and privileged populations.
- National Academies of Sciences, Engineering, and Medicine. 2019. *Minority Serving Institutions: America's Underutilized Resource for Strengthening the STEM Workforce.* Washington, DC: The National Academies Press. https://dor.org/10.17226/25257. This report notes that the United States needs to add 1 million STEM trained people to the workforce in the next decade. As the U.S. trends toward a non-white majority, there are millions of young people of color who remain strongly underrepresented in STEM. The report identifies minority serving institutions as a national resource that should be tapped to strengthen and diversify the STEM workforce.

The committee does not reproduce these studies in this report, but notes that they all urgently caution that technical education and training of the American workforce is not keeping up with the projected needs of an increasingly technical economy. If anything, the need in AMO is even greater due to its most direct connection to industry and application.

## FINDINGS AND RECOMMENDATIONS: REALIZING THE FULL POTENTIAL OF AMO SCIENCE

Several observations emerge from the studies undertaken that the committee highlights as the major findings of this chapter.

> **Finding:** Funding trends for AMO sciences show, after correction for inflation, little to no increase over the past decade, even as the number of AMO scientists in the United States has grown.
>
> **Recommendation: It is vital that the U.S. government continue to invest as a nation in curiosity-driven atomic, molecular, and optical science that enables a diverse set of scientific ideas and approaches to be explored.**
>
> **Finding:** As AMO laboratory programs grow more expensive to seed, the need for seeding the research of early career investigators is increasingly important.
>
> **Recommendation: The federal government should develop seed funding and portable fellowship grant models that support the transition of atomic, molecular, and optical theorists and experimentalists into faculty positions.**
>
> **Finding:** The number of theoretical AMO faculty positions in the United States is perennially low (dangerously low in certain subfields of AMO). AMO theory is an important component of AMO science and presents U.S. scientists with an opportunity to contribute to a vibrant and exciting field.
>
> **Recommendation: A vibrant theory program needs to be incentivized through funding opportunities, such as a portable fellowship grant program, and through a sustained campaign of educating and hiring theoretical AMO physicists.**
>
> **Finding:** The participation of women in AMO science is alarmingly low, with a large gap (relative to white males) in education and career advancement opportunities and outcomes. Systemic barriers to larger participation include societal and institutional biases toward these groups—often unintentional but nonetheless impactful—that lead to already small numbers declining at each career stage. The cultural norms and practices are seen as creating unwelcoming workplaces for these groups.

**Recommendation: Institutions receiving federal funding should implement stronger mechanisms to ensure a high standard of accountability in creating an inclusive workplace environment. Funding agencies may seek ways to incentivize this as well.**

**Finding:** There is little data on URMs, but from what we do have, it is clear that the numbers are extremely low. The committee has requested data on representation of URMs in federal funding and professional society membership, but very little information is available, in keeping with the very low numbers involved. Without high-quality demographic data, the underrepresentation of certain groups continues to be relegated to guesstimation and conjecture. What we do know is that a tremendous opportunity to engage large swaths of American society in AMO science—and in all STEM fields—is being squandered. The fraction of scientists in AMO from URM groups is dramatically smaller than the fraction in the general public, making it clear that those benefiting from education and funding opportunities in AMO do not reflect the demographic shifts in the nation, and that is a lost opportunity for the entire field.

**Recommendation: The entire AMO science enterprise should find a multitude of ways to tap into this growing talent pool.**

## CLOSING REMARKS

The excitement and tangible outcomes of AMO science, described in previous chapters, cannot be overstated. Overall U.S. participation—eminence even—in AMO science is strong, continuing to leverage investments of previous decades. However, new opportunities that require concerted and directed action to maintain U.S. eminence in the field are also highlighted. Few subfields of physics have greater impact on developing knowledge and technologies that profoundly influence society.

Even as the promise of AMO science continues to fuel research and innovation, it is apparent that education, workforce development, and career opportunities are not equitably impacting all members of society. Like so many areas of STEM, AMO science has very small representation of women and URMs. There are notable inequities and barriers for women and URMs, which are the result of cultural norms in science, unconscious and conscious biases that subtly and overtly devalue those who “don’t belong” in the dominant groups and cultures, harassing behaviors, lack of role models, and many other sociological factors. These pernicious sociological effects lead to inequitable outcomes and detract from the well-intentioned opportunities and support the AMO community tries to provide. There is much work to be done to create a more inclusive discipline that can harness the full power of a growingly diverse American society. The AMO community will grow even stronger by addressing these issues and seizing the opportunities to draw from a growing national talent pool.

Last, it is important to note that the sustained investments in AMO science in the United States are paying off as it continues to be a dynamic exciting field that is enabling fundamental exploration while also spawning new technologies, seeding invention and innovation, and having significant intellectual, societal, and economic impact.

# Appendixes

# A

# Statement of Task

The committee will be charged with producing a comprehensive report on the status and future directions of atomic, molecular, and optical (AMO) science. The committee's report shall:

1. Review the field of AMO science as a whole, emphasize recent accomplishments, and identify new opportunities and compelling scientific questions.
2. Use case studies in selected, nonprioritized fields in AMO science to describe the impact that AMO science has on other scientific fields, identify opportunities and challenges associated with pursuing research in these fields because of their interdisciplinary nature, and inform recommendations for addressing these challenges.
3. Identify the impacts of AMO science, now and in the near future, on emerging technologies and in meeting national needs.
4. Evaluate recent trends in investments in AMO research in the United States relative to similar research that is taking place internationally, and provide recommendations for either securing leadership in the United States for certain subfields of AMO science, where appropriate, or for enhancing collaboration and coordination of such research support, where appropriate.

5. Identify future workforce, societal, and educational needs for AMO science.
6. Make recommendations on how the U.S. research enterprise might realize the full potential of AMO science.

In carrying out its charge, the committee might consider issues such as the state of the AMO research community, international models for support and collaboration, and institutional and programmatic barriers.

# B

# Organization of the Report

The Statement of Task issued to the committee is reproduced in Appendix A. The content of the report is related to the tasks specifically. The first three tasks involve taking stock of recent developments in AMO science and identifying scientific opportunities for the coming decade. This is the bulk of the content of Chapters 2 through 7 of this report.

The remaining three tasks were aimed at evaluating funding and U.S. leadership, education and workforce training, and broader societal impacts of AMO research. These are the subject of the final chapter of this report.

# C

# Reprise of Past National Academies Reports on AMO Science

Since 1994, the National Academies of Sciences, Engineering, and Medicine has produced five reports examining various aspects of atomic, molecular, and optical (AMO) science: the 1994 decadal study, *Atomic, Molecular, and Optical Science: An Investment in the Future*; its supplement, *Atoms, Molecules, and Light: AMO Science Enabling the Future* (2002); the next decadal study, *Controlling the Quantum World: The Science of Atoms, Molecules, and Photons* (2007); *Optics and Photonics: Essential Technologies for Our Nation* (2013); and *Opportunities in Intense Ultrafast Lasers: Reaching for the Brightest Light* (2018). In this appendix, the committee considers the impact of these reports and the response to their report recommendations. To emphasize the historical nature of the issues discussed in this report, the committee also comments on the National Academies report *Atomic, Molecular, and Optical Physics* (1986).

## ATOMIC, MOLECULAR, AND OPTICAL SCIENCE: AN INVESTMENT IN THE FUTURE (1994)

In the 1994 study *Atomic, Molecular, and Optical Science: An Investment in the Future,* the panel arrived at three priorities for AMO science in the immediate future. Key facets of these recommendations were as follows:

- A pattern of support that maintains and enhances responsiveness of AMO science to national needs by ensuring the healthy diversity of the field and the strength of the core research;

- Research into highly promising new technologies for the control and manipulation of atoms, molecules, charged particles, and light; and
- Research into new and improved lasers and other advanced light sources.

Clearly, over the past 25 years the AMO community has seen rapid developments in laser technology, with a number of new emerging areas such as laser frequency combs, attosecond science, and coherent lights sources covering infrared to extreme ultraviolet. All areas of AMO science have been strongly impacted by these advances in laser technologies, which are reflected in the current report. The same is true for the control and manipulation of atoms, molecules, charged particles, and light. This is the core part of the AMO field, and researchers have seen revolutionary developments in capabilities of controlling individual particles. In fact, the community has moved beyond the point of single particle control and is now entering a new stage where these individually controlled particles are brought together to realize new experimental platforms for quantum information science, a field that is largely born out of AMO science in the mid-1990s.

The 1994 report also had some specific comments about the future of AMO science. Some science and technology trends foreseen at that time have in fact been realized.

Other predictions and trends have been more ambiguous, were avoided, or did not come to pass:

- A shift in federal funding away from defense agencies did not result in a serious erosion of basic AMO research. Department of Defense (DoD) support of fundamental science and AMO has remained strong, and continues to be vital to AMO science in the United States.
- The reorganization or reduction of industrial and federally funded laboratories may have been detrimental to the U.S. program in AMO science. Starting in the 1990s, large industrial laboratories devoted to AMO research have largely disappeared.

Some concerns noted in this 25-year-old report continue to resonate today and need addressing:

- Support for such essential core work in AMO science can still be negatively affected in times of limited funding by pressure to support research in more exotic areas.
- Many young scientists are still unable to find permanent positions.
- The U.S. AMO program is still losing ground relative to other countries, specifically those in Europe and China.

Other recommendations of the 1994 report are also still quite relevant:

- "The panel recommends that balanced involvement of the field in both basic and strategic research be maintained through the broad-based support structure that has developed for the field."
- "The panel recommends that the responsiveness and value of the field be further strengthened by developing closer ties with those areas and agencies that benefit and stand to further benefit from AMO science but that have not traditionally had strong links with the field, such as health, transportation, and environment. Institutions and agencies concerned with progress in these areas should also participate in the funding of AMO science."
- "The panel recommends that the federal agencies emphasize support for single investigators and small groups and rely on merit review for exploratory as well as strategic, goal-oriented basic research."

## ATOMS, MOLECULES, AND LIGHT: AMO SCIENCE ENABLING THE FUTURE (2002)

In 2002, a brief update to 1994 decadal, *Atoms, Molecules, and Light: AMO Science Enabling the Future,* was published. The intent was "(1) to delineate the connection between AMO discoveries and technological applications throughout society and (2) to highlight recent advances that will play an important role in shaping the landscape of scientific discovery and technological invention." This update was not tasked to produce additional findings, conclusions, or recommendations and was mainly a brochure; however, one key scientific highlight worth mentioning following its 1995 discovery was the Bose-Einstein condensate.

## CONTROLLING THE QUANTUM WORLD: THE SCIENCE OF ATOMS, MOLECULES, AND PHOTONS (2007)

In 2007, a subsequent full decadal study of AMO science was conducted: *Controlling the Quantum World: The Science of Atoms, Molecules, and Photons*. The report shows considerable awareness in linking AMO to national priorities—such as those outlined in the President's State of the Union in 2006 and the FY2007 budget request—and connecting with important watchwords for the future such as "coherence" and "control." Some of its key recommendations are still quite salient today and reinforce recommendations in this report:

- "The federal government should recognize the high cost of scientific instrumentation on research budgets and plan accordingly."

- "The funding agencies should reexamine their portfolios in theoretical research to ensure that the effort is at proper strength in workforce and funding levels."
- "The federal government should implement incentives to encourage more U.S. students, especially women and minorities, to study the physical sciences and take up careers in the field. It should continue to attract foreign students to study physical sciences and strongly encourage them to pursue their scientific careers in the United States."

The other key recommendations in the report may have been addressed, but to what extent is unclear:

- "In view of the critical importance of the physical sciences to national economic strength, health care, defense, and domestic security, the federal government should embark on a substantially increased investment program to improve education in the physical sciences and mathematics at all levels and to strengthen significantly the research effort."
- "AMO science will continue to make exceptional contributions to many areas of science and technology. The federal government should therefore support programs in AMO science across disciplinary boundaries and through a multiplicity of agencies."
- "Basic research is a vital component of the nation's defense strategy. The Department of Defense, therefore, should reverse recent declines in support for 6.1 [basic] research at its agencies."

The report also laid out a set of grand challenges with relevance to this report, as follows:

1. A revolution in precision measurement from a convergence of technologies in the control of the coherence of ultrafast lasers and ultracold atoms;
2. Potential contributions to fundamental problems in condensed-matter science and in plasma physics in ultracold AMO physics, especially after the development of coherent quantum gases;
3. Advances across AMO science, condensed-matter physics and materials research, chemistry, medicine, and defense-related science due to new high-intensity and short-wavelength light sources, such as X-ray free-electron lasers;
4. A revolution in imaging and coherent control of quantum processes—made possible by ultrafast light sources—in the internal motion of atoms within molecules;

5. Opportunities in molecular and photon science for atom-by-atom control of quantum structures with far-reaching societal applications; and
6. Multiple approaches to quantum computing and its potential application to data security and encryption.

The response to this report has been promising. In addition, at least two of the grand challenges above proved worthy of follow-up reports of their own: one on the future of optics and photonics (2013), and the other on high-intensity light sources (2018).

## OPTICS AND PHOTONICS: ESSENTIAL TECHNOLOGIES FOR OUR NATION (2013)

In *Optics and Photonics: Essential Technologies for Our Nation* (2013), optics and photonics are cited as a key enabling field for economic growth with a need for an authoritative vision. The report aims to (1) help policy makers and leaders decide on courses of action that can advance the economy of the United States, (2) provide visionary guidance and support for the future development of optics and photonics technology and applications, and (3) ensure a leadership role for the United States in these areas. Several field-specific recommendations are made in the report that are outside the scope of the present report; however, the first key recommendation is relevant:

- The committee recommends that the federal government develop an integrated initiative in photonics (similar in many respects to the National Nanotechnology Initiative) that seeks to bring together academic, industrial, and government researchers, managers, and policy makers to develop a more integrated approach to managing industrial and government photonics research and development (R&D) spending and related investments.

This key recommendation was responsible for the formation of the current National Photonics Initiative (NPI). The NPI, as stated on its website, has since become "a collaborative alliance among industry, academia and government seeking to raise awareness of photonics—the application of light—and drive U.S. funding and investment in five key photonics-driven fields critical to U.S. competitiveness and national security." Like the National Nanotechnology Initiative before it, the NPI has also become the model for other national science initiatives, such as the National Quantum Initiative.

## OPPORTUNITIES IN INTENSE ULTRAFAST LASERS: REACHING FOR THE BRIGHTEST LIGHT (2018)

In *Opportunities in Intense Ultrafast Lasers: Reaching for the Brightest Light* (2018), the committee was formed to assess the merit and extent of the scientific and technical advances that intense ultrafast lasers could afford the United States if such research was pursued. The concept for the report came out of the Committee on Atomic, Molecular, and Optical Sciences, a standing activity of the National Academies that operates under the auspices of the Board on Physics and Astronomy, and was motivated by three factors:

1. Recent breakthroughs in ultrafast high-power lasers and the underlying technology;
2. Nearly a decade of community network building in Europe with programs like Laserlab-Europe, Photonics21, and Horizon 2020, taking the advice recommended to U.S. agencies in the 2002 SAUUL report; and
3. Initiation of the first stage of the Extreme Light Infrastructure project to build several petawatt facilities at a few key sites in Europe.

Many useful field-specific recommendations resulted from this report and are actively being addressed across the federal agencies, including the National Science Foundation and the Department of Energy.

## ATOMIC, MOLECULAR, AND OPTICAL PHYSICS (1986)

The 1986 study *Atomic, Molecular, and Optical Physics,* chaired by Daniel Kleppner, was the first National Academies decadal survey of physics to include AMO science explicitly. The report identified promising research opportunities in AMO physics and made general recommendations in addition to many subfield-specific comments. Of particular note, the committee made overarching recommendations that connect with this report, including the following:

- Continued base support for experimental and theoretical research;
- Invitations for proposals from agencies to address the lack of theorists, possibly by creating centers, workshops, or summer schools where students and active theorists could come together for varying periods of time.

# D

# Committee Biographical Information

JUN YE, *Co-Chair*, is currently a fellow of JILA and a fellow of the National Institute of Standards and Technology (NIST) and a Physics Professor Adjoint at the University of Colorado, Boulder. At JILA, Dr. Ye's research focuses on the frontiers of light-matter interactions and includes precision measurement, quantum physics, ultracold matter, optical frequency metrology, and ultrafast science. Dr. Ye is a member of the National Academy of Sciences (NAS) and a recipient of many awards and honors, including the N. Ramsey Prize, the I. I. Rabi Award, a U.S. Presidential Rank (Distinguished) Award, four Gold Medals from the U.S. Commerce Department, Foreign Member of the Chinese Academy of Sciences, Frew fellow of the Australian Academy of Science, European Frequency and Time Forum Award, Carl Zeiss Research Award, William F. Meggers Award and Adolph Lomb Medal from the Optical Society of America, Arthur S. Flemming Award, Presidential Early Career Award for Scientists and Engineers, Friedrich Wilhem Bessel Award of the Alexander von Humboldt Foundation, Samuel Wesley Stratton Award, and Jacob Rabinow Award from NIST. Dr. Ye earned his Ph.D. in physics from the University of Colorado in 1997. He served as a member of the National Academies of Sciences, Engineering, and Medicine Committee on Atomic, Molecular, and Optical Sciences (CAMOS).

NERGIS MAVALVALA, *Co-Chair*, is the Curtis and Kathleen Marble Professor of Astrophysics at the Massachusetts Institute of Technology (MIT). Dr. Mavalvala is working on the detection of gravitational waves and quantum measurement science. She is a longtime member of the scientific team that announced in 2016 the first direct detection of gravitational waves from colliding black holes by the Laser Interferometer Gravitational-Wave Observatory (LIGO). In the quest for ever greater sensitivity in the LIGO detectors, Dr. Mavalvala has also conducted pioneering experiments on generation and application of exotic quantum states of light, and on laser cooling and trapping of macroscopic objects to enable observation of quantum phenomena, which usually manifest at the atomic scale, in human-scale systems. Dr. Mavalvala received a B.A. from Wellesley College and a Ph.D. from MIT. She was a postdoctoral fellow and research scientist at the California Institute of Technology before joining the physics faculty at MIT in 2002. She was appointed associate department head of physics in February 2015. Dr. Mavalvala is recipient of numerous honors, including a MacArthur "genius" award in 2010 and election to the NAS in 2017.

RAYMOND G. BEAUSOLEIL is the HPE Senior Fellow for Information and Quantum Systems at Hewlett Packard Labs. Dr. Beausoleil leads the Large-Scale Integrated Photonics Research Group at Hewlett Packard Labs, where he is responsible for research on the applications of optics at the micro/nanoscale to high-performance classical and quantum information processing. Dr. Beausoleil's research interests include solid-state laser physics, nonlinear optics, quantum optics, quantum information science and technology, nanophotonics, embedded computer algorithms, and image processing. He received his Ph.D. in physics from Stanford University.

PATRICIA M. DEHMER is the former deputy director for science programs in the Office of Science (SC) in the Department of Energy (DOE) and the former director of the Office of Basic Energy Sciences (BES) within SC. As the deputy director, Dr. Dehmer was the senior career science official in SC and was the acting director between Senate-confirmed Presidential appointees, most recently for 3 years from 2013 to 2015. As director of the BES Program, she was known for her broad support of physical science research and for the planning, design, and construction phases of a dozen major scientific construction projects totaling more than $3 billion. Previously, Dr. Dehmer was a distinguished fellow at Argonne National Laboratory with research activities in atomic, molecular, optical, and chemical physics. Since her retirement from federal service in 2016, she works as a management consultant with additional service on boards, science advisory committees, and professional society committees. During her federal service, Dr. Dehmer was awarded three Presidential Rank Awards and, in 2016, the James R. Schlesinger Award, the highest recognition in DOE, for management of SC's portfolio in the physical sciences and for outstanding management of DOE's largest-scale scientific construction projects. She is a fellow of the American Physical Society (APS) and the American Association for the Advancement of Science. Dr. Dehmer earned her Ph.D. in chemical physics from the University of Chicago. She served on and was vice chair of CAMOS.

LOUIS DIMAURO is the Edward E. and Sylvia Hagenlocker Chair of Physics at the Ohio State University (OSU). Before joining OSU in 2007, Dr. DiMauro was a senior scientist at Brookhaven National Laboratory. Dr. DiMauro's research interest is in experimental ultrafast and strong-field physics. His current work is focused on the generation, measurement, and application of attosecond X-ray pulses and the study of fundamental scaling of strong-field physics. Dr. DiMauro received his B.A. (1975) from Hunter College, CUNY, and his Ph.D. from the University of Connecticut in 1980. He was a postdoctoral fellow at SUNY at Stony Brook before arriving at AT&T Bell Laboratories in 1981.

METTE GAARDE is the Les and Dot Broussard Alumni Professor of Physics at Louisiana State University (LSU). Dr. Gaarde is an expert on the theory of ultrafast and strong-field laser-matter interactions in atomic, molecular, and solid systems. In particular, she is interested in the interplay between the microscopic (quantum) effects and the macroscopic (classical) effects that govern this interaction. Dr. Gaarde recently served on CAMOS, on the executive committee for the American Physical Society (APS) Division of Atomic, Molecular, and Optical Physics (DAMOP), and in the chair-line of the APS National Organizing Committee for the Conferences for Undergraduate Women in Physics. Dr. Gaarde earned her M.S. and Ph.D. in physics from Copenhagen University, Denmark, and was a research assistant professor at Lund University in Sweden before coming to LSU.

STEVEN GIRVIN is a Eugene Higgins Professor of Physics and Applied Physics at Yale University. Dr. Girvin is a theoretical physicist who studies the quantum mechanics of large collections of atoms, molecules, and electrons such as are found in superconductors, magnets, and transistors. Dr. Girvin is interested in quantum many-body physics and in quantum and classical phase transitions, particularly in disordered systems. Much of his work has been on the quantum Hall effect, but he has also worked on the superconductor-insulator transition, the vortex glass transition in high-Tc superconductors, superfluid helium in fractal aerogel, the Anderson localization problem, the Coulomb blockade problem in mesoscopic device physics, and on quantum spin chains. Dr. Girvin is a member of the NAS. He received his Ph.D. in 1977 from Princeton University.

CHRIS H. GREENE is a professor of physics at Purdue University. Previously, Dr. Greene was at Louisiana State University and the University of Colorado, Boulder. His research concentrates on theoretical atomic, molecular, and optical physics. Dr. Greene's expertise has been on novel treatments of few-body quantum systems, such as universal Efimov physics, ultra-long-range "trilobite" Rydberg molecules, collisions in Bose-Einstein condensates, atomic/molecular collision, and photo-absorption processes. He has served in the past as chair of JILA at the

University of Colorado. Dr. Greene received his Ph.D. in theoretical atomic physics from the University of Chicago in 1980. In 1981, he was a postdoctoral research associate at Stanford University.

TAEKJIP HA is Bloomberg Distinguished Professor of Biophysics and Biophysical Chemistry at Johns Hopkins University. He is also an investigator for the Howard Hughes Medical Institute. Dr. Ha's research is focused on pushing the limits of single-molecule detection methods to study complex biological systems. His group develops state-of-the-art biophysical techniques and applies them to study diverse protein-nucleic acid and protein-protein complexes, and mechanical perturbation and response of these systems both in vitro and in vivo. Dr. Ha is a member of the NAS. He received his B.S. (1990) from Seoul National University and Ph.D. from the University of California, Berkeley (1996), in physics.

MARK KASEVICH is a professor of applied physics at Stanford University. Prior to Stanford University, Dr. Kasevich was at Yale University. His research interests are centered on the development of quantum sensors of rotation and acceleration based on cold atoms (quantum metrology), the application of these sensors to the tests of general relativity, the investigation of many-body quantum effects in Bose-condensed vapors (including quantum simulation), and the investigation of ultrafast laser-induced phenomena. Dr. Kasevich graduated from Dartmouth College in 1985 with a B.A. in physics and received his Ph.D. in applied physics from Stanford University in 1992.

MICHAL LIPSON is the Eugene Higgins Professor in Electrical Engineering and a professor of applied physics at Columbia University. Prior to joining Columbia University, Dr. Lipson was the Given Foundation Professor of Engineering at Cornell University. Her research interests are in silicon photonics, invention of the GHz silicon modulator, novel on-chip nanophotonics devices, and novel micron-size photonic structures for light manipulation. In 2014, Dr. Lipson was named by Thomson Reuters as a top 1 percent highly cited researcher in the field of physics. She completed her B.S., M.S., and Ph.D. degrees in physics at the Technion (Israel Institute of Technology), followed by a postdoctoral position at MIT in the Materials Science Department until 2001.

MIKHAIL LUKIN is a professor of physics at Harvard University, where he is also a co-director of the Harvard-MIT Center for Ultracold Atoms. Dr. Lukin's research interests include quantum optics, quantum control of atomic and nanoscale solid-state systems, quantum metrology, nanophotonics, and quantum information science. He has co-authored more than 300 technical papers and has received a number of awards, including the Alfred P. Sloan Fellowship, the David and Lucile

Packard Fellowship for Science and Engineering, the NSF Career Award, the Adolph Lomb Medal of the Optical Society of America, the AAAS Newcomb Cleveland Prize, the APS I.I.Rabi Prize, the Vannevar Bush Faculty Fellowship, the Julius Springer Prize for Applied Physics, and the Willis E. Lamb Award for Laser Science and Quantum Optics. Dr. Lukin is a member of the NAS. He received his Ph.D. from Texas A&M University in 1998.

A. MARJATTA LYYRA is a professor of physics at Temple University. Prior to joining Temple University, Dr. Lyyra was a research scientist at the University of Iowa. Her field of interest is experimental atomic, molecular, and optical physics with an emphasis on high resolution spectroscopy, quantum optics, and chemical dynamics using the "dressed states" tool of Autler-Townes splittings to manipulate molecular dynamics. She is a fellow of the American Physical Society and a fellow of the Optical Society of America. Dr. Lyyra received her B.S. and M.S. degrees from the University of Helsinki, Finland (1972, 1974), and her Ph.D. from the University of Stockholm, Sweden, in 1979.

PETER J. REYNOLDS is a senior research scientist with the Army Research Office (ARO) and an Adjunct Professor of Physics at North Carolina State University. He serves as a scientific advisor across the Army, helping to set research directions, particularly in the physical sciences, and seeks out emerging areas for investment both intra- and extramurally. Prior to this he served as the head of physics at ARO, and before that as program manager for Atomic & Molecular Physics. Prior to joining ARO, Dr. Reynolds was at the Office of Naval Research running the Atomic & Molecular Physics program there from 1988-2003. From 1980-1988 he was a staff scientist at the Lawrence Berkeley Laboratory. His background is computational and theoretical physics approaches in statistical mechanics, particularly in renormalization group theory and Monte Carlo methods for both classical and quantum systems. He has received the U.S. Presidential Rank Award as a Distinguished Senior Scientist in 2015, and is a long-time fellow of the American Physical Society. Dr. Reynolds obtained his Ph.D. in theoretical condensed-matter physics from MIT in 1979 and an A.B. in physics from the University of California, Berkeley, in 1971.

MARIANNA SAFRONOVA is a professor of physics at the University of Delaware and an adjunct fellow of the Joint Quantum Institute, NIST, and the University of Maryland. Dr. Safronova is currently the chair-elect of APS DAMOP and a member of the *Physical Review A* editorial board (2012-2018). Her diverse research interests include the study of fundamental symmetries and the search for physics beyond the Standard Model of elementary particles and fundamental interactions; development of high-precision methodologies for calculating atomic properties and exploring their applications; atomic clocks, ultracold atoms, and quantum information; long-range interactions; superheavy atoms; highly charged ions; atomic anions; and other topics. In 2001, Dr. Safronova received her Ph.D. from the University of Notre Dame.

PETER ZOLLER is a professor of physics at the University of Innsbruck, Austria, and scientific director for the Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences. Dr. Zoller's interest and expertise are in the field of theoretical quantum optics, in particular the description of interaction of light with matter, and various aspects of quantum noise. During the past 10 years, the focus of his work has been on the interface between quantum optics and quantum information, and condensed-matter physics with cold atoms. Dr. Zoller is a member of the NAS and received his Ph.D. in physics from the University of Innsbruck.

# E

# Data Solicitation and Collection

## DATA SOLICITATION FROM FEDERAL AGENCIES

Nine federal agencies (Air Force Office of Scientific Research, Army Research Office, Defense Advanced Research Projects Agency, Department of Energy, Intelligence Advanced Research Projects Activity, the National Aeronautics and Space Administration, National Institute of Standards and Technology, National Science Foundation, and the Office of Naval Research,) that fund atomic, molecular, and optical (AMO) research were asked to respond to the following questions.

### Questions on Funding

In order to understand the impact of federal funding on AMO research, the AMO2020 committee is seeking the answers to the following questions:

1. What is the absolute number of dollars spent on AMO research each year over the past decade at your agency?
2. What is the distribution of grant size each year for the past 10 years?
   The above questions aim to understand if funding for AMO sciences has remained robust over the past decade. We would appreciate if the relevant program officer would aggregate AMO spending across all programs at the agency.
3. Over the past decade, how many awards go to grantees each year as a function of the grantee's time past PhD. We can divide this into three time spans: 5 years after PhD, 10 years after PhD, and beyond 10 years.

> This is to understand opportunities for early career scientists to secure federal funding for their research. These questions are posed to federal funding agencies that fund or support atomic, molecular, and optical (AMO) research.

### Questions on Interagency Activities and Partnerships

As AMO research grows increasingly cross-disciplinary in nature, the committee is interested in understanding how funding is distributed between large-scale research and single-PI groups. To this end, we pose the following questions to the funding agencies.

1. If your agency support centers or large-group efforts in AMO science, what is the size of the awards per year for centers relative to the total budget spent on AMO each year?
2. Briefly describe the extent to which your agency supports interdisciplinary activities that include AMO science.
3. Briefly describe the extent of industrial participation in AMO awards and how this has changed over the past 10 years.

## DEMOGRAPHIC QUESTIONNAIRE

In order to ensure that opportunities in AMO sciences are accessible to a diverse set of practitioners, the committee would like to understand the level of participation for women and underrepresented minorities. To this end, we pose the following questions to professional societies that fund or support atomic, molecular, and optical (AMO) research.

1. Over the past 10 years, what is the total number of Ph.D. degrees granted at U.S. institutions each year?
2. Of that total, how many degrees each year were granted in an AMO-related field?
3. Of the degrees granted in an AMO-related field, how many each year were granted to
    a. Women
    b. Underrepresented minorities

These data will be used to make a plot that shows the number of AMO-related Ph.D.s relative to total physics Ph.D.s granted as a function of time, as well as the fraction of those AMO-related degrees that go to women and underrepresented minorities.

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# Acronyms

| | |
|---|---|
| 1D | one-dimensional |
| 2D | two-dimensional |
| 3D | three-dimensional |
| | |
| AFM | atomic force microscopy |
| AFOSR | Air Force Office of Scientific Research |
| ALMA | Atacama large millimeter/submillimeter array |
| ALP | axion-like particle |
| AMO | atomic, molecular, and optical |
| APS | American Physical Society |
| APV | atomic parity violation |
| ARIADNE | axion resonant interaction detection experiment |
| ARO | Army Research Office |
| ATAS | attosecond transient absorption spectroscopy |
| ATI | above threshold ionization |
| | |
| BASE | baryon-antibaryon symmetry experiment |
| BEC | Bose-Einstein condensate |
| BES | Basic Energy Sciences |
| BI | Bell inequality |
| BSM | beyond the Standard Model |

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|---|---|
| CAMOS | Committee on Atomic, Molecular, and Optical Sciences |
| CASPEr | cosmic axion spin precession experiment |
| CDI | coherent diffractive imaging |
| CEP | carrier envelope phase |
| CFT | conformal field theory |
| CI | configuration interaction |
| CI | conical intersection |
| CMOS | complementary metal oxide semiconductor |
| CMP | condensed-matter physics |
| COLTRIMS | cold target recoil ion momentum spectroscopy |
| COT | commercial off-the-shelf technology |
| CPA | chirped pulse amplification |
| cQED | cavity quantum electrodynamics |
| CSGB | chemical sciences, geosciences, and biosciences |
| CSR | cryogenic storage ring |
| CSS | coherent spin state |
| DAMOP | Division of Atomic, Molecular, and Optical Physics |
| DARPA | Defense Advanced Research Projects Agency |
| DFG | degenerate Fermi gas |
| DFT | density functional theory |
| DIQKD | device independent quantum key distribution |
| DM | dark matter |
| DMRG | density-matrix renormalization group |
| DoD | Department of Defense |
| DOE | Department of Energy |
| EBIT | electron-beam ion trap |
| EDM | electric dipole moment |
| eEDM | electron EDM |
| EIT | electromagnetically induced transparency |
| ELI | extreme light infrastructure |
| EM | electromagnetic |
| EPR | electron paramagnetic resonance |
| ETH | eigenstate thermalization hypothesis |
| EWP | electron wave packet |
| FB | Floquet-Bloch |
| FEL | free-electron laser |
| FRET | fluorescence resonance energy transfer |

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|---|---|
| GHZ | Greenberger-Horn-Zeilinger |
| GNOME | global network of optical magnetometers to search for exotic physics |
| GPU | graphical processing unit |
| GPV | group velocity distribution |
| GR | general theory of relativity |
| GW | gravitational wave |
| HCI | highly charged ion |
| HEP | high energy physics |
| HHG | high harmonic generation |
| HHS | high harmonic spectroscopy |
| HL | Heisenberg limit |
| ITAMP | Institute for Theoretical Atomic, Molecular, and Optical Physics |
| ITER | International Thermonuclear Experimental Reactor |
| JWST | James Webb space telescope |
| LCLS | Linac Coherent Light Source |
| LF | light filamentation |
| LHC | Large Hadron Collider |
| LIBS | laser-induced breakdown spectroscopy |
| LIED | laser-induced electron diffraction |
| LIGO | Laser Interferometer Gravitational-Wave Observatory |
| LINAC | linear accelerator |
| LISA | Laser Interferometer Space Antenna |
| LLI | local Lorentz invariance |
| LV | LLI violation |
| MBL | many-body localization |
| MBPT | many-body perturbation theory |
| MCSCF | multiconfiguration self-consistent field |
| MFM | magnetic force microscope |
| ML | machine learning |
| ML | mode-locked |
| MPS | mathematical and physical sciences |
| MRFM | magnetic resonance force microscopy |
| MRI | magnetic resonance imaging |
| MRS | Materials Research Society |
| MTB | magnetotactic bacterium |

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|---|---|
| NASA | National Aeronautics and Space Administration |
| NIR | near-infrared |
| NIST | National Institute of Standards and Technology |
| NMR | nuclear magnetic resonance |
| NNI | National Nanotechnology Initiative |
| NPI | National Photonics Initiative |
| NQI | National Quantum Initiative |
| NRC | National Research Council |
| NSF | National Science Foundation |
| NV | nitrogen vacancy |
| OCT | optical coherence tomography |
| OFC | optical frequency comb |
| OM | optomechanics |
| ONR | Office of Naval Research |
| OPM | optically pumped magnetometer |
| OPO | optical parametric oscillator |
| OSTP | Office of Science and Technology Policy |
| PAH | polyaromatic hydrocarbon |
| PDK | process design kit |
| PEA | phase estimation algorithm |
| PI | principal investigator |
| PIC | photonic integrated circuit |
| PQS | programmable quantum simulator |
| QAOA | quantum approximate optimization algorithm |
| QCD | quantum chromodynamics |
| QED | quantum electrodynamics |
| QIP | quantum information processing |
| QIS | quantum information science |
| QIST | quantum information science and technology |
| QKD | quantum key distribution |
| QMC | quantum Monte Carlo |
| QND | quantum nondemolition |
| QR | quantum repeater |
| QRNG | quantum random number generator |
| qubit | quantum bit |
| R&D | research and development |
| RABBITT | reconstruction of attosecond beating by interference of two-photon transitions |

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|---|---|
| RC | reservoir computing |
| RNG | random number generator |
| RV | radial velocity |
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| SASE | self amplified stimulated emission |
| SERF | spin-exchange relaxation free |
| SiV | silicon vacancy |
| SLAC | Stanford Linear Accelerator Center |
| SM | Standard Model |
| SOC | spin-orbit coupling |
| SOFIA | Stratospheric Observatory for Infrared Astronomy |
| SPI | single-particle imaging |
| SQCAMscope | scanning quantum cryogenic atom microscope |
| SQL | standard quantum limit |
| SQUID | superconducting quantum interference device |
| SSS | squeezed spin state |
| STED | stimulated emission depletion |
| STEM | science, technology, engineering, and mathematics |
| | |
| TDDFT | time-dependent density functional theory |
| TEM | transmission electron microscope |
| TMDC | transition metal dichalcogenide |
| | |
| UED | ultrafast electron diffraction |
| URM | underrepresented minorities |
| | |
| VMI | velocity map imaging |
| VQE | variational quantum eigensolver |
| VQS | variational quantum simulation |
| VUV | vacuum ultraviolet |
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| WIMP | weakly interacting massive particle |
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| XFEL | X-ray free-electron laser |
| XUV | extreme ultraviolet |